Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:21 PM UTC

PDB ID	:	1HJK / pdb_00001hjk
Title	:	ALKALINE PHOSPHATASE MUTANT H331Q
Authors	:	Murphy, J.E.; Stec, B.; Ma, L.; Kantrowitz, E.R.
Deposited on	:	1997-05-30
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

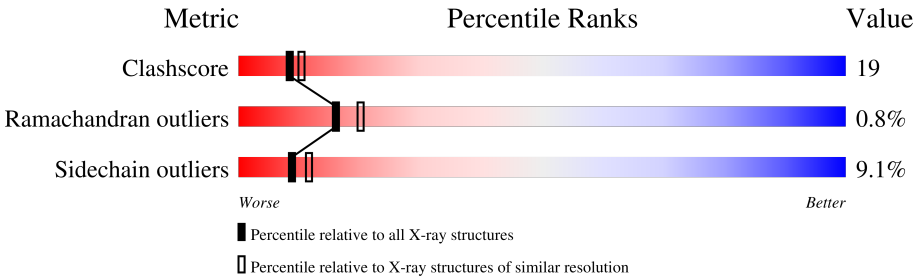
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	56% 36% 7%
1	B	449	54% 38% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	P	S	0	0	0
			3307	2041	580	673	1	12			
1	B	449	Total	C	N	O	P	S	0	0	0
			3307	2041	580	673	1	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	SEP	SER	modified residue	UNP P00634
A	331	GLN	HIS	engineered mutation	UNP P00634
B	102	SEP	SER	modified residue	UNP P00634
B	331	GLN	HIS	engineered mutation	UNP P00634

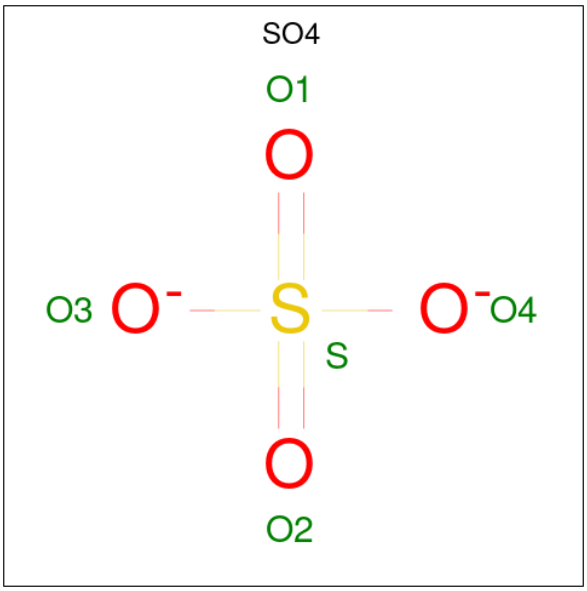
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	231	Total O 231 231	0	0
5	B	283	Total O 283 283	0	0

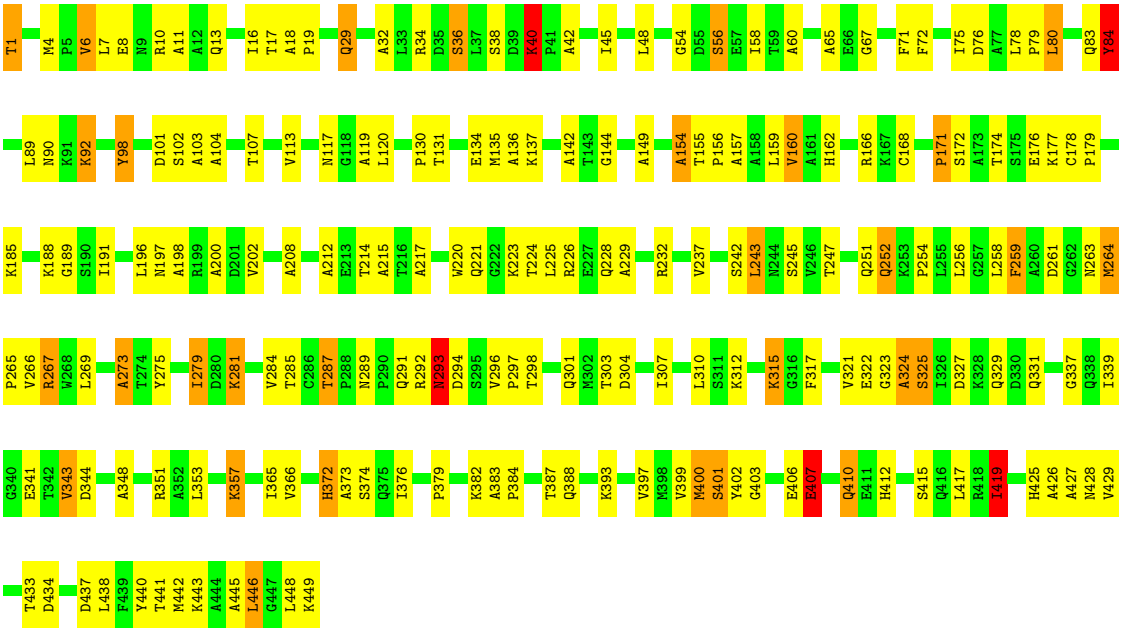
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

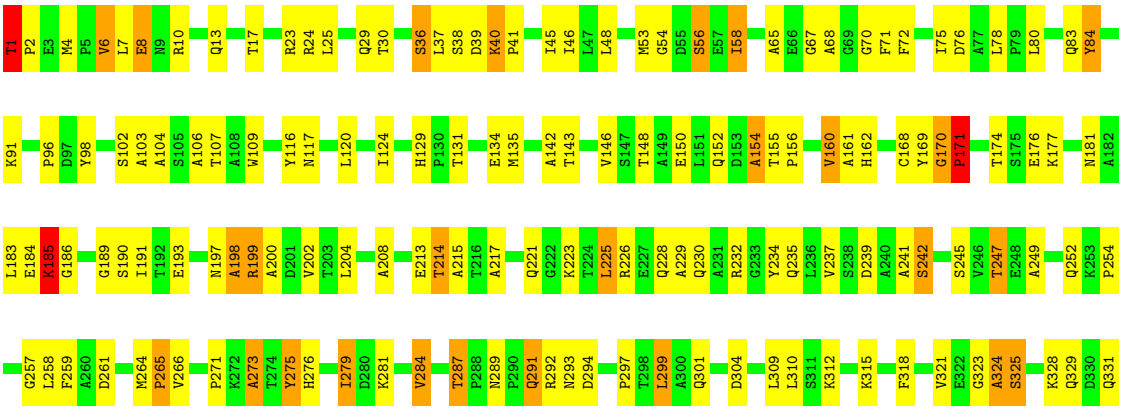
• Molecule 1: ALKALINE PHOSPHATASE

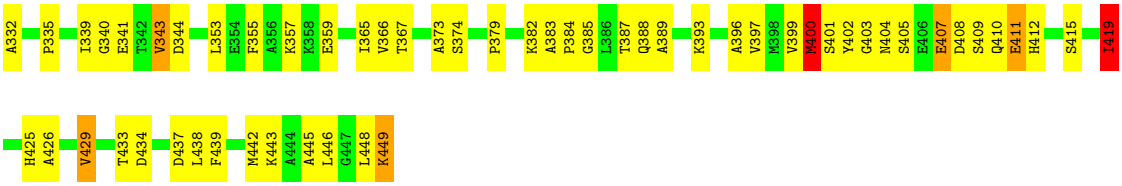
Chain A:



• Molecule 1: ALKALINE PHOSPHATASE

Chain B:




A332
P335
I339
G340
E341
T342
V343
D344
L353
E354
F355
A356
K357
K358
E359
I365
V366
T367
A373
S374
P379
K382
A383
P384
G385
L386
T387
Q388
A389
K393
A396
V397
M398
V399
M400
S401
Y402
G403
N404
S405
E406
E407
D408
S409
Q410
E411
H412
S415
I419
H425
A426
V429
T433
D434
D437
L438
F439
M442
K443
A444
A445
L446
G447
L448
K449

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	195.52Å 167.86Å 77.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	90.0 (8.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7144	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, SO4, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.22	12/3350 (0.4%)	1.48	50/4546 (1.1%)
1	B	1.21	2/3350 (0.1%)	1.48	48/4546 (1.1%)
All	All	1.21	14/6700 (0.2%)	1.48	98/9092 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	MET	SD-CE	-15.77	1.40	1.79
1	A	400	MET	SD-CE	-11.12	1.51	1.79
1	A	372	HIS	CD2-NE2	6.80	1.45	1.37
1	B	58	ILE	CA-CB	6.51	1.62	1.54
1	A	89	LEU	CA-C	-6.40	1.44	1.52
1	A	374	SER	C-O	-6.21	1.16	1.23
1	A	18	ALA	CA-CB	-5.95	1.46	1.53
1	A	376	ILE	CA-CB	5.92	1.61	1.54
1	A	113	VAL	CA-CB	5.90	1.62	1.54
1	A	11	ALA	CA-CB	-5.82	1.44	1.53
1	A	348	ALA	CA-CB	-5.65	1.44	1.53
1	A	157	ALA	CA-CB	-5.62	1.44	1.53
1	A	196	LEU	CA-C	5.36	1.59	1.52
1	A	264	MET	CG-SD	-5.16	1.67	1.80

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	ASN	N-CA-C	12.60	137.63	110.80
1	A	324	ALA	N-CA-C	11.29	123.34	111.14
1	B	324	ALA	N-CA-C	10.17	122.13	111.14
1	B	325	SER	N-CA-C	8.64	123.48	113.19
1	A	1	THR	CA-C-N	8.32	130.24	119.84
1	A	1	THR	C-N-CA	8.32	130.24	119.84
1	B	98	TYR	N-CA-C	8.21	121.14	111.71
1	A	98	TYR	N-CA-C	8.00	122.14	112.38
1	B	185	LYS	N-CA-C	-7.96	104.02	112.93
1	B	343	VAL	CB-CA-C	-7.88	101.50	112.14
1	A	273	ALA	N-CA-C	-7.84	100.16	110.43
1	A	325	SER	N-CA-C	7.72	122.38	113.19
1	B	65	ALA	N-CA-C	7.55	122.26	112.89
1	A	373	ALA	N-CA-C	7.50	120.91	111.69
1	B	383	ALA	CA-C-N	7.41	127.05	119.19
1	B	383	ALA	C-N-CA	7.41	127.05	119.19
1	A	293	ASN	N-CA-C	7.28	126.30	110.80
1	A	412	HIS	N-CA-C	-7.22	100.99	110.53
1	B	67	GLY	CA-C-O	-7.19	117.27	122.23
1	B	412	HIS	N-CA-C	-7.17	101.07	110.53
1	B	265	PRO	N-CA-C	7.09	122.20	111.14
1	B	154	ALA	N-CA-C	6.87	119.36	111.11
1	B	299	LEU	N-CA-C	-6.87	103.88	111.36
1	A	13	GLN	N-CA-C	6.86	118.75	111.28
1	B	294	ASP	N-CA-C	-6.83	103.63	112.23
1	A	65	ALA	N-CA-C	6.82	121.35	112.89
1	B	67	GLY	N-CA-C	-6.81	104.66	112.29
1	B	373	ALA	N-CA-C	6.80	120.06	111.69
1	B	323	GLY	N-CA-C	-6.79	97.09	113.18
1	B	1	THR	CA-C-N	6.65	128.15	119.84
1	B	1	THR	C-N-CA	6.65	128.15	119.84
1	B	411	GLU	N-CA-C	6.61	119.82	110.50
1	B	200	ALA	N-CA-C	-6.53	98.98	109.96
1	A	374	SER	N-CA-C	6.49	119.39	110.24
1	B	273	ALA	N-CA-C	-6.47	101.37	110.50
1	A	67	GLY	N-CA-C	-6.47	105.04	112.29
1	A	185	LYS	N-CA-C	-6.46	105.27	113.02
1	A	200	ALA	N-CA-C	-6.43	100.96	110.48
1	B	374	SER	N-CA-C	6.41	119.28	110.24
1	A	29	GLN	N-CA-C	6.41	120.31	112.23
1	A	383	ALA	CA-C-N	6.40	125.97	119.19
1	A	383	ALA	C-N-CA	6.40	125.97	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	GLN	N-CA-C	6.40	119.07	111.33
1	B	7	LEU	N-CA-C	-6.39	100.44	109.96
1	A	189	GLY	N-CA-C	6.28	119.39	111.85
1	A	265	PRO	N-CA-C	6.21	120.94	111.19
1	B	170	GLY	CA-C-N	6.20	127.59	119.84
1	B	170	GLY	C-N-CA	6.20	127.59	119.84
1	A	79	PRO	N-CA-C	6.18	121.67	113.57
1	B	161	ALA	N-CA-C	6.11	119.61	110.14
1	A	267	ARG	N-CA-C	6.07	117.90	111.28
1	A	317	PHE	N-CA-C	6.05	118.05	108.79
1	B	53	MET	N-CA-C	6.00	118.95	108.52
1	A	259	PHE	N-CA-C	5.99	119.54	112.72
1	A	136	ALA	N-CA-C	-5.92	104.74	111.14
1	A	154	ALA	N-CA-C	5.89	118.18	111.11
1	A	40	LYS	CB-CA-C	-5.85	98.65	110.17
1	B	225	LEU	N-CA-C	-5.78	105.06	111.36
1	B	78	LEU	CA-C-N	5.71	125.24	119.19
1	B	78	LEU	C-N-CA	5.71	125.24	119.19
1	A	410	GLN	N-CA-C	-5.68	101.23	110.20
1	A	296	VAL	N-CA-C	5.68	113.17	107.55
1	B	150	GLU	N-CA-C	-5.65	101.28	110.20
1	B	189	GLY	N-CA-C	5.64	118.62	111.85
1	A	298	THR	N-CA-C	-5.59	103.53	110.41
1	A	178	CYS	CA-C-N	5.54	124.74	118.97
1	A	178	CYS	C-N-CA	5.54	124.74	118.97
1	A	323	GLY	N-CA-C	-5.51	100.12	113.18
1	B	419	ILE	N-CA-C	-5.49	100.16	108.17
1	B	6	VAL	CB-CA-C	-5.47	103.26	110.98
1	B	449	LYS	N-CA-C	5.44	126.22	111.00
1	A	351	ARG	N-CA-C	-5.42	105.27	111.07
1	B	429	VAL	CB-CA-C	-5.42	104.97	110.88
1	A	419	ILE	N-CA-C	-5.40	100.28	108.17
1	A	294	ASP	N-CA-C	-5.38	105.84	112.90
1	B	291	GLN	N-CA-C	5.37	119.55	113.15
1	A	322	GLU	N-CA-C	5.37	117.65	108.90
1	A	75	ILE	N-CA-C	5.31	120.38	109.34
1	A	172	SER	N-CA-C	5.30	118.20	111.69
1	A	32	ALA	N-CA-C	-5.28	104.78	111.11
1	A	343	VAL	CB-CA-C	-5.24	105.17	111.88
1	A	406	GLU	N-CA-C	-5.22	105.65	112.23
1	B	315	LYS	N-CA-C	5.22	118.75	112.38
1	B	396	ALA	CA-C-N	-5.22	115.08	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	396	ALA	C-N-CA	-5.22	115.08	122.34
1	A	428	ASN	N-CA-C	5.19	121.86	110.80
1	A	243	LEU	N-CA-C	-5.17	105.64	111.28
1	B	343	VAL	N-CA-CB	5.16	117.55	110.54
1	A	130	PRO	N-CA-C	5.13	118.55	110.80
1	B	252	GLN	N-CA-C	-5.10	107.72	114.04
1	A	315	LYS	N-CA-C	5.10	118.60	112.38
1	B	8	GLU	N-CA-CB	5.10	117.97	110.33
1	B	198	ALA	N-CA-C	5.03	118.68	112.54
1	A	281	LYS	CA-C-N	5.03	126.14	120.66
1	A	281	LYS	C-N-CA	5.03	126.14	120.66
1	A	266	VAL	CA-C-N	5.00	126.99	120.28
1	A	266	VAL	C-N-CA	5.00	126.99	120.28
1	B	181	ASN	N-CA-C	-5.00	107.85	114.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	TYR	Sidechain
1	A	84	TYR	Sidechain
1	B	275	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3307	0	3249	115	2
1	B	3307	0	3249	150	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	231	0	0	7	3
5	B	283	0	0	9	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7144	0	6498	251	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ALA:HB3	1:A:221:GLN:HA	1.44	0.98
1:A:292:ARG:O	1:A:293:ASN:HB2	1.71	0.91
1:A:60:ALA:HB1	1:A:400:MET:HE3	1.54	0.90
1:B:291:GLN:HB3	5:B:721:HOH:O	1.71	0.89
1:B:135:MET:HE1	1:B:443:LYS:HD2	1.61	0.82
1:A:38:SER:OG	1:A:40:LYS:HG2	1.83	0.79
1:B:199:ARG:NH2	1:B:254:PRO:HG3	1.97	0.78
1:B:160:VAL:HG12	1:B:198:ALA:HB3	1.65	0.77
1:B:215:ALA:HB3	1:B:221:GLN:HA	1.64	0.77
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.68	0.76
1:A:45:ILE:HD12	1:A:446:LEU:HD13	1.68	0.75
1:B:38:SER:OG	1:B:40:LYS:HG2	1.89	0.72
1:B:408:ASP:HA	5:B:490:HOH:O	1.88	0.72
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.70	0.72
1:B:160:VAL:CG1	1:B:198:ALA:HB3	2.20	0.71
1:B:10:ARG:HB2	1:B:71:PHE:CE1	2.27	0.70
1:A:135:MET:HE1	1:A:443:LYS:HD2	1.73	0.70
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.72	0.70
1:A:60:ALA:HB1	1:A:400:MET:CE	2.22	0.70
1:A:259:PHE:HB2	1:A:264:MET:HE3	1.72	0.70
1:B:4:MET:HG2	1:B:36:SER:HA	1.74	0.69
1:B:328:LYS:HG2	5:B:708:HOH:O	1.91	0.69
1:A:259:PHE:CB	1:A:264:MET:HE3	2.23	0.68
1:A:438:LEU:HG	1:A:442:MET:HE2	1.74	0.68
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.59	0.68
1:A:56:SER:HA	1:B:415:SER:HB2	1.75	0.67
1:B:297:PRO:HA	1:B:301:GLN:OE1	1.94	0.67
1:B:276:HIS:CG	1:B:279:ILE:HD11	2.30	0.67
1:A:168:CYS:SG	1:A:174:THR:HA	2.35	0.66
1:B:259:PHE:HB2	1:B:264:MET:HE3	1.77	0.66
1:B:29:GLN:HA	1:B:29:GLN:NE2	2.10	0.65
1:B:160:VAL:HG12	1:B:198:ALA:CB	2.27	0.65
1:B:168:CYS:SG	1:B:177:LYS:HB2	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:HIS:CD2	1:B:445:ALA:HA	2.32	0.64
1:A:45:ILE:CD1	1:A:446:LEU:HD13	2.28	0.64
1:A:176:GLU:HG3	1:A:177:LYS:HG3	1.79	0.64
1:A:247:THR:O	1:A:312:LYS:NZ	2.31	0.64
1:B:247:THR:O	1:B:312:LYS:NZ	2.31	0.63
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.28	0.63
1:B:193:GLU:HG2	1:B:225:LEU:HD11	1.79	0.62
1:B:343:VAL:HG23	1:B:344:ASP:N	2.13	0.62
1:B:171:PRO:HG2	1:B:225:LEU:HD21	1.82	0.61
1:A:197:ASN:HB3	5:A:462:HOH:O	2.01	0.61
5:A:563:HOH:O	1:B:29:GLN:HG3	2.01	0.61
1:B:146:VAL:HG22	1:B:204:LEU:HB2	1.83	0.60
1:B:249:ALA:HB2	1:B:309:LEU:HD13	1.82	0.60
1:A:331:GLN:HA	1:A:410:GLN:HB2	1.82	0.60
1:A:384:PRO:HB2	1:B:384:PRO:HB2	1.84	0.60
1:A:269:LEU:HB2	1:A:287:THR:HG22	1.83	0.60
1:B:176:GLU:HG3	1:B:177:LYS:HG2	1.82	0.60
1:A:4:MET:HG2	1:A:36:SER:HA	1.85	0.59
1:A:226:ARG:O	1:A:229:ALA:HB3	2.02	0.59
1:A:289:ASN:O	1:A:292:ARG:HG2	2.02	0.59
1:A:214:THR:HG22	1:A:224:THR:N	2.17	0.58
1:A:228:GLN:O	1:A:232:ARG:HG3	2.02	0.58
1:A:415:SER:CB	1:B:56:SER:HA	2.33	0.58
1:A:426:ALA:O	1:A:429:VAL:HG22	2.03	0.58
1:B:276:HIS:ND1	1:B:279:ILE:HD11	2.17	0.58
1:A:297:PRO:HA	1:A:301:GLN:OE1	2.04	0.58
1:B:217:ALA:O	1:B:221:GLN:HB3	2.03	0.58
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.87	0.57
1:B:91:LYS:HD2	1:B:116:TYR:CD1	2.40	0.56
1:A:29:GLN:HG3	5:B:622:HOH:O	2.05	0.56
1:A:220:TRP:O	1:A:223:LYS:HG2	2.06	0.56
1:B:259:PHE:CB	1:B:264:MET:HE3	2.35	0.56
1:A:267:ARG:HD2	1:A:344:ASP:HB2	1.89	0.55
1:B:353:LEU:O	1:B:357:LYS:HB2	2.05	0.55
1:B:279:ILE:HD12	1:B:382:LYS:HE2	1.89	0.54
1:B:434:ASP:O	1:B:437:ASP:HB2	2.07	0.54
1:A:212:ALA:HB2	5:A:651:HOH:O	2.07	0.54
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.43	0.53
1:B:331:GLN:HE21	1:B:409:SER:HB3	1.73	0.53
1:A:415:SER:HB3	1:B:56:SER:HA	1.90	0.53
1:B:142:ALA:HB1	1:B:310:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.89	0.53
1:A:6:VAL:CG2	1:A:357:LYS:HD3	2.39	0.53
1:B:152:GLN:HB2	1:B:169:TYR:CD2	2.44	0.53
1:B:148:THR:HG23	1:B:299:LEU:HD13	1.90	0.53
1:B:104:ALA:HB2	1:B:117:ASN:HA	1.90	0.53
1:B:40:LYS:HB2	1:B:41:PRO:CD	2.39	0.52
1:A:208:ALA:HB2	1:A:258:LEU:HB3	1.91	0.52
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.91	0.52
1:B:197:ASN:HA	1:B:232:ARG:NH2	2.24	0.52
1:B:226:ARG:HH11	1:B:226:ARG:CG	2.22	0.52
1:A:440:TYR:CE2	1:B:23:ARG:HD2	2.44	0.52
1:B:199:ARG:CZ	1:B:254:PRO:HG3	2.39	0.52
1:B:275:TYR:HA	1:B:385:GLY:O	2.10	0.52
1:A:417:LEU:C	1:A:417:LEU:HD12	2.34	0.52
1:B:148:THR:CG2	1:B:299:LEU:HD13	2.39	0.52
1:B:284:VAL:HG23	1:B:389:ALA:O	2.10	0.52
1:A:407:GLU:HG2	5:A:643:HOH:O	2.10	0.51
1:A:403:GLY:O	1:B:384:PRO:HD2	2.10	0.51
1:B:23:ARG:NH1	5:B:623:HOH:O	2.43	0.51
1:A:120:LEU:O	1:A:162:HIS:HA	2.10	0.51
1:A:48:LEU:HB2	1:A:366:VAL:HG22	1.93	0.51
1:A:279:ILE:HD12	1:A:382:LYS:HE2	1.91	0.51
1:A:393:LYS:O	1:A:393:LYS:HG2	2.10	0.51
1:A:438:LEU:O	1:A:442:MET:HG3	2.10	0.51
1:B:48:LEU:HB2	1:B:366:VAL:HG22	1.93	0.51
1:B:91:LYS:HD2	1:B:116:TYR:CE1	2.45	0.51
1:A:60:ALA:CB	1:A:400:MET:HE3	2.33	0.51
1:A:215:ALA:CB	1:A:221:GLN:HA	2.28	0.51
1:A:217:ALA:C	1:A:221:GLN:HB3	2.35	0.51
1:B:72:PHE:HB2	1:B:76:ASP:OD2	2.11	0.51
1:B:214:THR:HG22	1:B:223:LYS:C	2.35	0.51
1:B:438:LEU:HG	1:B:442:MET:HE2	1.93	0.51
1:B:438:LEU:O	1:B:442:MET:HG3	2.11	0.51
1:A:104:ALA:HB2	1:A:117:ASN:HA	1.92	0.50
1:B:170:GLY:HA2	1:B:190:SER:OG	2.11	0.50
1:A:387:THR:HG22	1:A:401:SER:HB2	1.94	0.50
1:B:120:LEU:O	1:B:162:HIS:HA	2.11	0.50
1:B:289:ASN:O	1:B:292:ARG:HG2	2.10	0.50
1:A:267:ARG:HG2	1:A:292:ARG:NH1	2.27	0.50
1:A:202:VAL:HG23	1:A:310:LEU:HD21	1.94	0.50
1:A:214:THR:HG22	1:A:223:LYS:C	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLU:O	1:B:225:LEU:HD23	2.12	0.49
1:B:45:ILE:HD12	1:B:446:LEU:HD12	1.93	0.49
1:B:343:VAL:CG2	1:B:344:ASP:N	2.74	0.49
1:B:103:ALA:HA	1:B:154:ALA:HB1	1.95	0.49
1:A:103:ALA:HB1	1:A:119:ALA:O	2.13	0.49
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.94	0.49
1:B:199:ARG:NH2	1:B:254:PRO:HD3	2.29	0.48
1:B:335:PRO:HD2	1:B:388:GLN:OE1	2.13	0.48
1:A:415:SER:HB2	1:B:56:SER:HA	1.95	0.48
1:A:419:ILE:HG12	1:A:429:VAL:HB	1.95	0.48
1:A:303:THR:O	1:A:307:ILE:HG13	2.13	0.48
1:B:405:SER:HB2	1:B:411:GLU:HG2	1.94	0.48
1:A:6:VAL:HG21	1:A:357:LYS:HD3	1.94	0.48
1:A:137:LYS:HE3	1:A:251:GLN:OE1	2.14	0.48
1:A:177:LYS:C	1:A:179:PRO:HD3	2.39	0.48
1:B:287:THR:HG22	1:B:287:THR:O	2.14	0.48
1:A:160:VAL:HG12	1:A:198:ALA:CB	2.44	0.47
1:A:237:VAL:HG11	1:A:243:LEU:HA	1.95	0.47
1:B:217:ALA:C	1:B:221:GLN:HB3	2.39	0.47
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.95	0.47
1:B:443:LYS:HG3	1:B:448:LEU:HB3	1.96	0.47
1:A:214:THR:HG22	1:A:224:THR:HA	1.97	0.47
1:A:149:ALA:HA	1:A:263:ASN:OD1	2.14	0.47
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.97	0.47
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.45	0.47
1:B:340:GLY:O	1:B:343:VAL:HG22	2.14	0.47
1:B:266:VAL:HG22	5:B:705:HOH:O	2.15	0.46
1:A:252:GLN:N	1:A:252:GLN:CD	2.73	0.46
1:B:239:ASP:OD2	1:B:241:ALA:HB3	2.15	0.46
1:B:355:PHE:CZ	1:B:359:GLU:HG3	2.50	0.46
1:B:199:ARG:NH2	1:B:254:PRO:CG	2.74	0.46
1:A:353:LEU:O	1:A:357:LYS:HB2	2.16	0.46
1:B:143:THR:HA	1:B:318:PHE:O	2.16	0.46
1:B:228:GLN:OE1	1:B:232:ARG:NH1	2.48	0.46
1:A:220:TRP:CH2	1:A:232:ARG:HD2	2.51	0.46
1:B:214:THR:CG2	1:B:223:LYS:C	2.89	0.46
1:A:42:ALA:HB2	1:A:445:ALA:HB1	1.98	0.46
1:A:407:GLU:HA	1:A:407:GLU:OE1	2.16	0.46
1:B:54:GLY:O	1:B:58:ILE:HG13	2.16	0.45
1:B:275:TYR:CE1	1:B:276:HIS:CD2	3.05	0.45
1:A:339:ILE:O	1:A:343:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:O	1:B:229:ALA:HB3	2.16	0.45
1:A:10:ARG:HB2	1:A:71:PHE:CE1	2.51	0.45
1:A:168:CYS:O	1:A:191:ILE:HG13	2.17	0.45
1:A:252:GLN:C	1:A:254:PRO:HD3	2.42	0.45
1:A:259:PHE:HB3	1:A:264:MET:HE3	1.97	0.45
1:B:29:GLN:O	1:B:30:THR:C	2.60	0.45
1:B:331:GLN:HA	1:B:410:GLN:HB2	1.97	0.45
1:A:188:LYS:HE3	5:A:542:HOH:O	2.16	0.45
1:B:184:GLU:HG2	1:B:185:LYS:N	2.31	0.45
1:A:7:LEU:HD21	5:A:601:HOH:O	2.17	0.45
1:A:29:GLN:NE2	1:A:29:GLN:HA	2.30	0.45
1:B:1:THR:HA	1:B:2:PRO:HD2	1.71	0.45
1:A:372:HIS:CE1	5:A:667:HOH:O	2.70	0.45
1:B:387:THR:HG22	1:B:401:SER:HB2	1.99	0.45
1:A:142:ALA:HB1	1:A:310:LEU:HD22	1.98	0.44
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.48	0.44
1:B:202:VAL:HG23	1:B:310:LEU:HD21	1.98	0.44
1:B:106:ALA:O	1:B:107:THR:C	2.60	0.44
1:B:109:TRP:O	1:B:439:PHE:HB2	2.17	0.44
1:B:273:ALA:HA	1:B:388:GLN:HB2	1.99	0.44
1:B:404:ASN:ND2	1:B:411:GLU:HB2	2.31	0.44
1:A:54:GLY:O	1:A:58:ILE:HG13	2.17	0.44
1:B:183:LEU:O	1:B:186:GLY:N	2.49	0.44
1:A:425:HIS:CD2	1:A:445:ALA:HA	2.52	0.44
1:B:208:ALA:HB2	1:B:258:LEU:HB3	1.98	0.44
1:A:80:LEU:HD12	1:A:427:ALA:HA	1.99	0.44
1:B:325:SER:HB2	1:B:341:GLU:HG3	2.00	0.44
1:B:339:ILE:HD11	1:B:400:MET:CE	2.47	0.44
1:B:24:ARG:NH1	1:B:70:GLY:O	2.46	0.44
1:B:129:HIS:O	1:B:162:HIS:HE1	2.01	0.44
1:A:144:GLY:HA2	1:A:202:VAL:O	2.18	0.44
1:B:46:ILE:HG22	1:B:48:LEU:HD22	2.00	0.44
1:B:237:VAL:HG13	1:B:242:SER:HB2	2.00	0.44
1:B:124:ILE:HD13	1:B:124:ILE:HG21	1.79	0.44
1:B:367:THR:HB	1:B:419:ILE:HD12	1.98	0.44
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.86	0.43
1:B:228:GLN:HG2	1:B:232:ARG:HD3	2.00	0.43
1:A:56:SER:HA	1:B:415:SER:CB	2.45	0.43
1:A:434:ASP:O	1:A:437:ASP:HB2	2.19	0.43
1:A:72:PHE:HB2	1:A:76:ASP:OD2	2.18	0.43
1:B:190:SER:OG	1:B:193:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:OG1	1:A:134:GLU:HG3	2.18	0.43
1:B:155:THR:HB	1:B:156:PRO:HD3	1.99	0.43
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.80	0.43
1:B:226:ARG:CG	1:B:226:ARG:NH1	2.80	0.43
1:B:228:GLN:CG	1:B:232:ARG:HD3	2.49	0.43
1:B:271:PRO:HD2	1:B:284:VAL:HG11	2.00	0.43
1:A:214:THR:HG22	1:A:224:THR:CA	2.49	0.43
1:B:39:ASP:O	1:B:425:HIS:CE1	2.72	0.43
1:A:4:MET:HE3	1:A:4:MET:HB2	1.84	0.42
1:A:269:LEU:HB2	1:A:287:THR:CG2	2.47	0.42
1:B:29:GLN:NE2	1:B:29:GLN:CA	2.78	0.42
1:B:234:TYR:CD1	1:B:254:PRO:HG2	2.54	0.42
1:B:329:GLN:O	1:B:332:ALA:HB3	2.18	0.42
1:A:34:ARG:HG3	1:B:37:LEU:HD12	2.01	0.42
1:B:131:THR:HG23	1:B:134:GLU:OE1	2.19	0.42
1:A:101:ASP:OD2	1:A:166:ARG:NH1	2.52	0.42
1:B:10:ARG:O	1:B:24:ARG:HD3	2.19	0.42
1:B:168:CYS:O	1:B:191:ILE:HG13	2.19	0.42
1:B:184:GLU:C	1:B:186:GLY:H	2.25	0.42
1:B:214:THR:HG22	1:B:223:LYS:O	2.19	0.42
1:A:325:SER:HB2	1:A:341:GLU:HG3	2.02	0.42
1:B:129:HIS:O	1:B:162:HIS:CE1	2.73	0.42
1:B:247:THR:HB	5:B:528:HOH:O	2.20	0.42
1:A:329:GLN:HG3	1:A:337:GLY:C	2.44	0.42
1:B:332:ALA:HB2	5:B:519:HOH:O	2.20	0.42
1:A:155:THR:HB	1:A:156:PRO:HD3	2.02	0.41
1:A:284:VAL:HG12	1:A:285:THR:N	2.34	0.41
1:A:103:ALA:HA	1:A:154:ALA:HB1	2.02	0.41
1:B:276:HIS:O	1:B:279:ILE:HG12	2.20	0.41
1:B:449:LYS:HB3	1:B:449:LYS:HE2	1.88	0.41
1:A:98:TYR:HE1	1:B:68:ALA:HB2	1.85	0.41
1:A:78:LEU:HD13	1:A:366:VAL:HB	2.02	0.41
1:B:341:GLU:O	1:B:344:ASP:HB3	2.21	0.41
1:B:393:LYS:O	1:B:393:LYS:HG2	2.20	0.41
1:A:83:GLN:HA	1:A:417:LEU:O	2.21	0.41
1:A:84:TYR:HA	1:A:433:THR:O	2.21	0.41
1:A:273:ALA:HA	1:A:388:GLN:HB2	2.02	0.41
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.70	0.41
1:B:148:THR:OG1	1:B:324:ALA:HB3	2.20	0.41
1:B:264:MET:HB3	1:B:265:PRO:HD2	2.03	0.41
1:B:168:CYS:SG	1:B:174:THR:HA	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PRO:HD2	1:B:403:GLY:O	2.21	0.41
1:B:84:TYR:HA	1:B:433:THR:O	2.21	0.41
1:B:10:ARG:NH2	1:B:29:GLN:OE1	2.54	0.41
1:B:426:ALA:O	1:B:429:VAL:HG22	2.21	0.41
1:B:393:LYS:NZ	5:B:674:HOH:O	2.54	0.40
1:A:10:ARG:HB2	1:A:71:PHE:CD1	2.56	0.40
1:A:19:PRO:HG3	1:B:129:HIS:CE1	2.57	0.40
1:A:83:GLN:HE21	1:B:83:GLN:HE21	1.69	0.40
1:B:91:LYS:HB2	1:B:116:TYR:CB	2.51	0.40
1:B:407:GLU:HB3	1:B:408:ASP:H	1.70	0.40
1:A:16:ILE:HD11	1:B:96:PRO:HD3	2.03	0.40
1:A:90:ASN:OD1	1:A:92:LYS:HB3	2.22	0.40
1:B:237:VAL:O	1:B:257:GLY:HA2	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:517:HOH:O	5:B:517:HOH:O[4_556]	0.64	1.56
5:A:542:HOH:O	5:A:542:HOH:O[3_656]	1.12	1.08
5:A:638:HOH:O	5:A:638:HOH:O[3_656]	1.22	0.98
1:A:188:LYS:NZ	5:A:495:HOH:O[3_656]	1.82	0.38
1:A:291:GLN:NE2	5:B:537:HOH:O[6_555]	2.03	0.17

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/449 (99%)	417 (94%)	26 (6%)	3 (1%)	18	23
1	B	446/449 (99%)	421 (94%)	21 (5%)	4 (1%)	14	17
All	All	892/898 (99%)	838 (94%)	47 (5%)	7 (1%)	16	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	407	GLU
1	B	407	GLU
1	B	75	ILE
1	B	199	ARG
1	B	171	PRO
1	A	171	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	339/339 (100%)	305 (90%)	34 (10%)	7 9
1	B	339/339 (100%)	311 (92%)	28 (8%)	10 14
All	All	678/678 (100%)	616 (91%)	62 (9%)	9 11

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	6	VAL
1	A	8	GLU
1	A	17	THR
1	A	36	SER
1	A	40	LYS
1	A	56	SER
1	A	80	LEU
1	A	84	TYR
1	A	92	LYS
1	A	107	THR
1	A	160	VAL
1	A	171	PRO
1	A	225	LEU
1	A	242	SER
1	A	245	SER

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Mol	Chain	Res	Type
1	A	252	GLN
1	A	256	LEU
1	A	261	ASP
1	A	279	ILE
1	A	281	LYS
1	A	287	THR
1	A	293	ASN
1	A	304	ASP
1	A	315	LYS
1	A	327	ASP
1	A	357	LYS
1	A	397	VAL
1	A	401	SER
1	A	407	GLU
1	A	419	ILE
1	A	441	THR
1	A	446	LEU
1	A	449	LYS
1	B	1	THR
1	B	6	VAL
1	B	8	GLU
1	B	17	THR
1	B	25	LEU
1	B	36	SER
1	B	40	LYS
1	B	56	SER
1	B	80	LEU
1	B	84	TYR
1	B	160	VAL
1	B	171	PRO
1	B	185	LYS
1	B	214	THR
1	B	230	GLN
1	B	235	GLN
1	B	242	SER
1	B	245	SER
1	B	247	THR
1	B	261	ASP
1	B	279	ILE
1	B	281	LYS
1	B	284	VAL
1	B	287	THR

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Mol	Chain	Res	Type
1	B	304	ASP
1	B	397	VAL
1	B	400	MET
1	B	419	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	329	GLN
1	A	350	GLN
1	A	391	ASN
1	A	410	GLN
1	B	83	GLN
1	B	230	GLN
1	B	252	GLN
1	B	331	GLN
1	B	412	HIS
1	B	425	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	B	102	2,1	8,9,10	0.90	0	7,12,14	3.74	2 (28%)
1	SEP	A	102	2,1	8,9,10	0.92	0	7,12,14	5.15	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	102	2,1	-	3/6/8/10	-
1	SEP	A	102	2,1	-	0/6/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	SEP	OG-CB-CA	-13.28	95.22	108.14
1	B	102	SEP	OG-CB-CA	-9.49	98.91	108.14
1	A	102	SEP	O3P-P-OG	2.29	112.64	106.67
1	B	102	SEP	O3P-P-OG	2.11	112.16	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	102	SEP	CB-OG-P-O3P
1	B	102	SEP	CB-OG-P-O1P
1	B	102	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	456	-	4,4,4	0.96	0	6,6,6	0.38	0
4	SO4	A	456	-	4,4,4	0.48	0	6,6,6	0.54	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.