



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:12 AM UTC

PDB ID : 3B97 / pdb_00003b97
Title : Crystal Structure of human Enolase 1
Authors : Kang, H.J.; Jung, S.K.; Kim, S.J.; Chung, S.J.
Deposited on : 2007-11-02
Resolution : 2.20 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

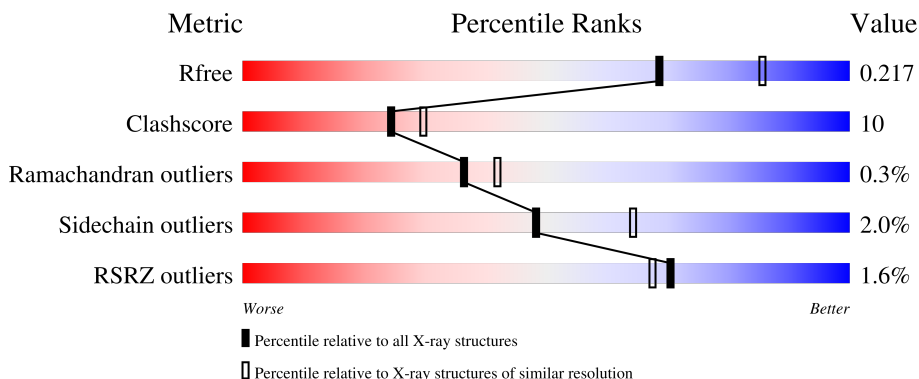
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	3% 79% 19% .
1	B	433	% 78% 20% .
1	C	433	% 77% 20% .
1	D	433	% 77% 20% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13815 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.

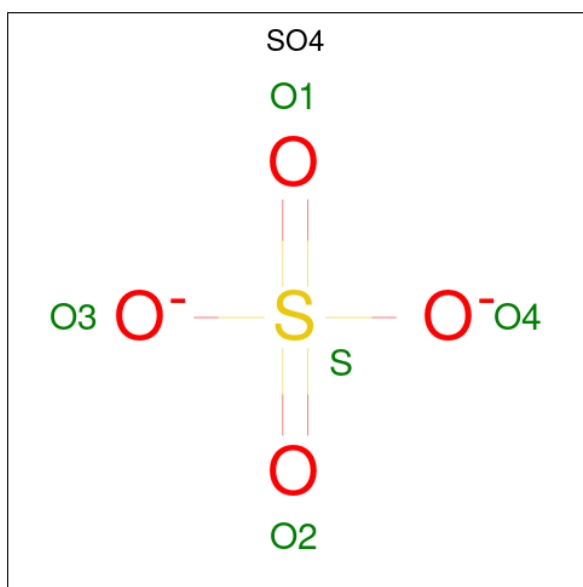
- Molecule 1 is a protein called Alpha-enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3297	2081	570	632	14			
1	B	432	Total	C	N	O	S	0	0	0
			3297	2081	570	632	14			
1	C	433	Total	C	N	O	S	0	0	0
			3307	2087	572	634	14			
1	D	431	Total	C	N	O	S	0	0	0
			3292	2078	569	631	14			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

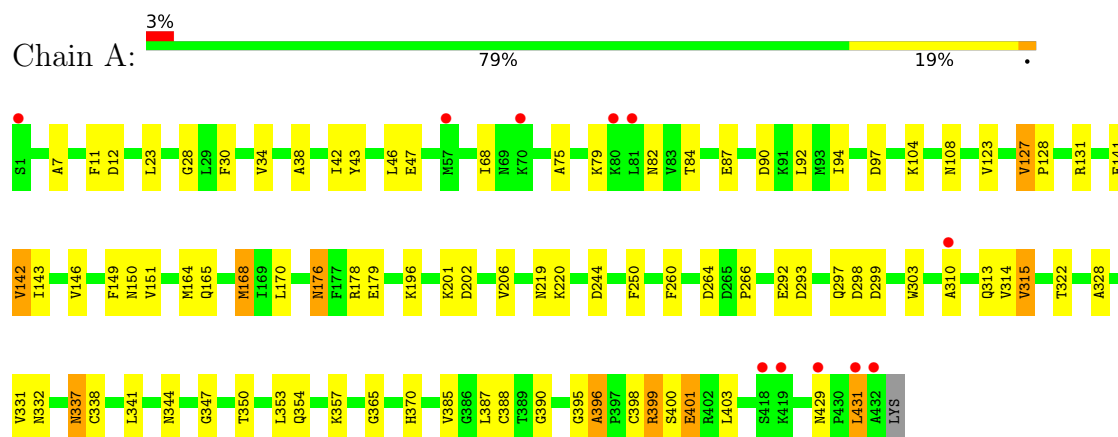
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	171	Total	O	0	0
			171	171		
4	C	132	Total	O	0	0
			132	132		
4	D	98	Total	O	0	0
			98	98		

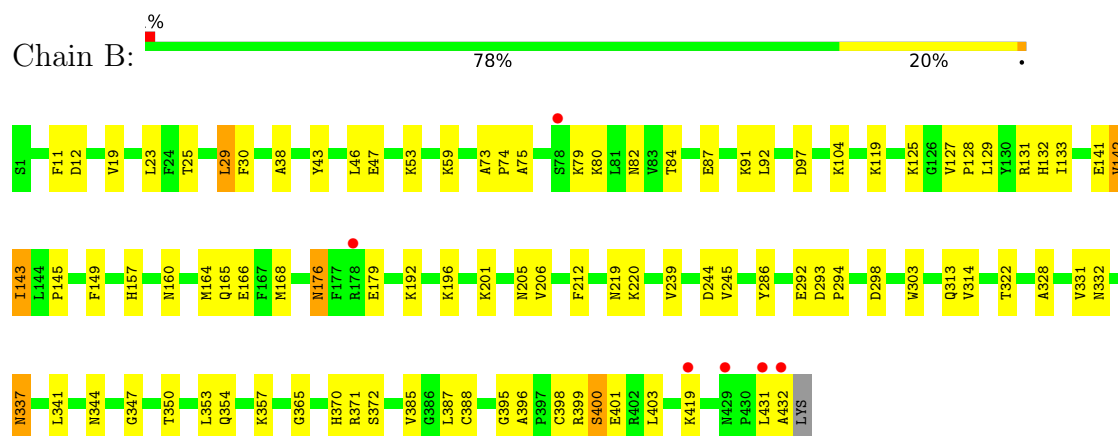
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

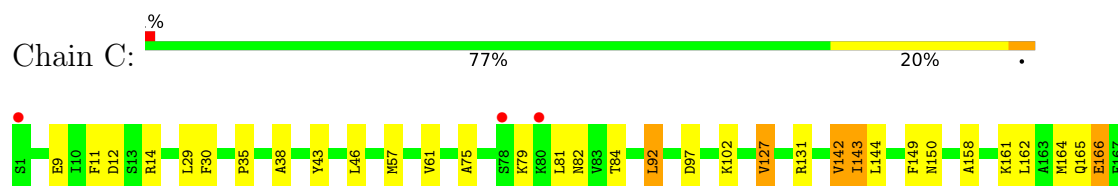
• Molecule 1: Alpha-enolase

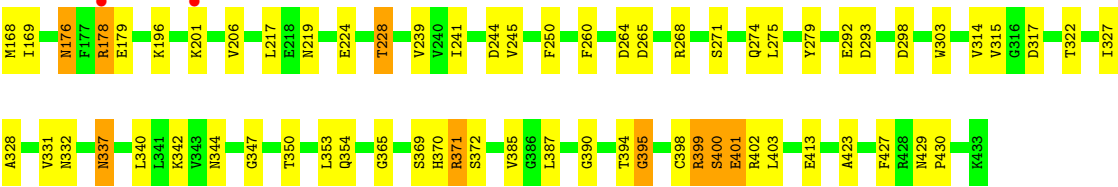


• Molecule 1: Alpha-enolase

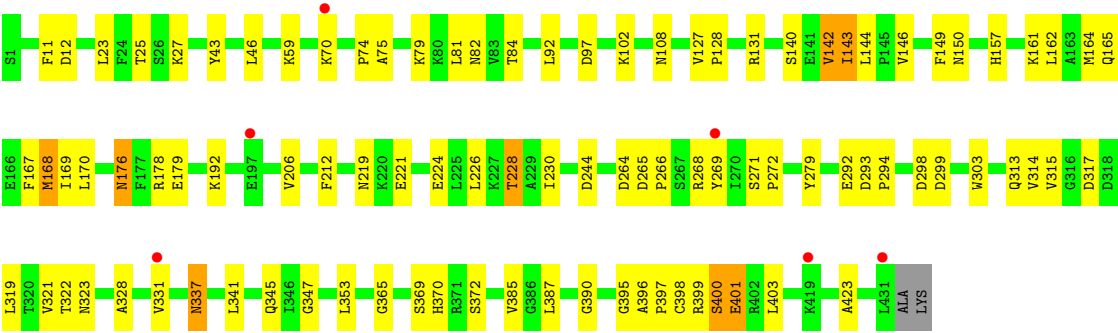
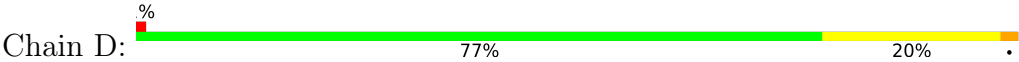


• Molecule 1: Alpha-enolase





● Molecule 1: Alpha-enolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	192.80Å 192.80Å 65.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.20) 97.0 (50.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.00 (at 2.20Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.184 , 0.217 0.184 , 0.217	Depositor DCC
R_{free} test set	6107 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13815	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.52	0/3352	1.03	20/4523 (0.4%)
1	B	0.49	0/3352	0.99	18/4523 (0.4%)
1	C	0.49	0/3362	1.01	19/4534 (0.4%)
1	D	0.46	0/3347	0.98	17/4516 (0.4%)
All	All	0.49	0/13413	1.00	74/18096 (0.4%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ALA	N-CA-C	12.10	124.21	111.14
1	B	165	GLN	N-CA-C	9.93	121.86	111.14
1	D	146	VAL	N-CA-C	-9.82	100.19	108.63
1	D	165	GLN	N-CA-C	9.01	120.79	110.97
1	A	165	GLN	N-CA-C	8.99	120.84	111.14
1	C	165	GLN	N-CA-C	8.81	120.49	111.07
1	B	395	GLY	N-CA-C	8.47	120.68	112.04
1	A	146	VAL	N-CA-C	-8.06	101.70	108.63
1	A	395	GLY	N-CA-C	7.67	119.87	112.04
1	C	429	ASN	CA-C-N	7.44	127.46	119.28
1	C	429	ASN	C-N-CA	7.44	127.46	119.28
1	D	365	GLY	N-CA-C	-6.96	101.89	112.89
1	C	347	GLY	N-CA-C	6.64	124.64	115.27
1	B	365	GLY	N-CA-C	-6.53	102.33	112.85
1	D	315	VAL	N-CA-C	6.49	117.64	108.36
1	A	365	GLY	N-CA-C	-6.39	102.79	112.89
1	C	395	GLY	N-CA-C	6.35	118.52	112.04
1	B	239	VAL	N-CA-C	6.33	116.97	108.11
1	C	365	GLY	N-CA-C	-6.26	103.02	112.60
1	C	38	ALA	N-CA-C	-6.24	104.63	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	VAL	N-CA-C	6.18	118.78	109.20
1	C	46	LEU	N-CA-C	6.11	118.57	109.59
1	C	239	VAL	N-CA-C	6.08	116.88	108.12
1	B	46	LEU	N-CA-C	6.08	118.53	109.59
1	C	315	VAL	N-CA-C	6.08	117.05	108.36
1	D	206	VAL	N-CA-C	6.05	118.58	109.20
1	C	430	PRO	N-CA-C	6.05	121.82	113.65
1	A	46	LEU	N-CA-C	6.04	118.47	109.59
1	D	395	GLY	N-CA-C	6.01	119.60	112.33
1	A	347	GLY	N-CA-C	5.98	123.70	115.27
1	D	347	GLY	N-CA-C	5.96	123.68	115.27
1	C	401	GLU	N-CA-C	-5.93	105.89	113.01
1	B	143	ILE	N-CA-C	5.89	116.84	108.42
1	C	400	SER	N-CA-C	5.88	119.93	112.87
1	D	400	SER	N-CA-C	5.86	119.53	112.38
1	B	347	GLY	N-CA-C	5.82	123.38	115.00
1	A	315	VAL	N-CA-C	5.82	116.68	108.36
1	B	47	GLU	N-CA-C	-5.80	99.07	108.41
1	B	400	SER	N-CA-C	5.78	119.43	112.38
1	A	206	VAL	N-CA-C	5.75	117.96	108.99
1	C	369	SER	N-CA-C	5.73	118.11	109.23
1	C	371	ARG	N-CA-C	-5.73	100.80	109.85
1	B	401	GLU	N-CA-C	-5.71	106.16	113.01
1	A	401	GLU	N-CA-C	-5.71	106.16	113.01
1	B	205	ASN	N-CA-C	-5.70	103.17	110.53
1	D	401	GLU	N-CA-C	-5.67	106.21	113.01
1	B	206	VAL	N-CA-C	5.63	117.93	109.20
1	D	369	SER	N-CA-C	5.63	117.96	109.23
1	D	140	SER	N-CA-C	-5.61	106.56	113.41
1	A	38	ALA	N-CA-C	-5.61	105.22	112.68
1	D	168	MET	N-CA-C	5.60	119.19	110.17
1	A	299	ASP	N-CA-C	-5.51	103.02	110.68
1	A	151	VAL	N-CA-C	5.49	120.60	113.07
1	A	396	ALA	N-CA-C	-5.49	100.98	109.87
1	A	28	GLY	N-CA-C	5.44	118.55	110.60
1	B	371	ARG	N-CA-C	-5.43	101.27	109.85
1	A	400	SER	N-CA-C	5.38	118.95	112.38
1	B	59	LYS	N-CA-C	5.36	118.83	112.72
1	B	25	THR	N-CA-C	-5.35	101.31	108.86
1	C	158	ALA	N-CA-C	5.28	117.41	109.23
1	A	168	MET	N-CA-C	5.25	118.29	109.95
1	D	46	LEU	N-CA-C	5.24	117.29	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ALA	N-CA-C	-5.18	106.04	112.93
1	D	345	GLN	N-CA-C	-5.17	106.49	112.89
1	D	59	LYS	N-CA-C	5.16	119.26	112.92
1	D	397	PRO	N-CA-C	-5.15	105.53	112.48
1	C	427	PHE	N-CA-C	5.11	117.59	111.71
1	A	34	VAL	N-CA-C	5.09	113.43	107.89
1	A	47	GLU	N-CA-C	-5.08	100.23	108.41
1	C	241	ILE	N-CA-C	5.06	116.64	108.85
1	A	264	ASP	N-CA-C	5.05	117.67	110.24
1	B	396	ALA	N-CA-C	-5.04	101.71	109.87
1	D	299	ASP	N-CA-C	-5.03	104.57	111.81
1	B	19	VAL	N-CA-C	5.01	116.03	109.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3297	0	3327	60	0
1	B	3297	0	3327	66	0
1	C	3307	0	3340	78	0
1	D	3292	0	3321	77	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	193	0	0	2	0
4	B	171	0	0	3	0
4	C	132	0	0	0	0
4	D	98	0	0	1	0
All	All	13815	0	13315	263	0

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 10.

All (263) 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:C:196:LYS:HE3	1:C:201:LYS:HG2	1.47	0.96
1:C:166:GLU:HG3	1:C:244:ASP:HB3	1.49	0.94
1:A:196:LYS:HE3	1:A:201:LYS:HG2	1.53	0.90
1:C:314:VAL:H	1:C:337:ASN:HD21	1.21	0.85
1:B:353:LEU:HD22	1:B:387:LEU:HD21	1.61	0.83
1:C:403:LEU:HD13	1:D:12:ASP:O	1.80	0.82
1:A:353:LEU:HD22	1:A:387:LEU:HD21	1.64	0.79
1:D:79:LYS:HG3	1:D:92:LEU:HD11	1.65	0.78
1:D:353:LEU:HD22	1:D:387:LEU:HD21	1.65	0.77
1:D:314:VAL:H	1:D:337:ASN:HD21	1.33	0.76
1:C:314:VAL:H	1:C:337:ASN:ND2	1.84	0.76
1:A:314:VAL:H	1:A:337:ASN:HD21	1.35	0.74
1:D:75:ALA:O	1:D:79:LYS:HG2	1.89	0.73
1:B:176:ASN:ND2	1:B:179:GLU:H	1.86	0.73
1:B:350:THR:O	1:B:354:GLN:HG3	1.90	0.72
1:C:75:ALA:O	1:C:79:LYS:HG2	1.90	0.71
1:D:176:ASN:ND2	1:D:178:ARG:HG3	2.06	0.71
1:B:142:VAL:HG13	1:B:385:VAL:CG1	2.21	0.70
1:D:314:VAL:H	1:D:337:ASN:ND2	1.89	0.70
1:A:328:ALA:O	1:A:331:VAL:HG22	1.93	0.69
1:B:82:ASN:ND2	1:B:84:THR:H	1.91	0.69
1:D:176:ASN:ND2	1:D:179:GLU:H	1.91	0.67
1:B:97:ASP:O	1:B:104:LYS:HE2	1.94	0.67
1:C:178:ARG:HG2	1:C:413:GLU:OE1	1.95	0.67
1:D:127:VAL:HG21	1:D:131:ARG:HG2	1.75	0.67
1:A:266:PRO:HG3	4:A:550:HOH:O	1.95	0.66
1:B:82:ASN:ND2	1:B:84:THR:OG1	2.28	0.66
1:D:244:ASP:HA	1:D:292:GLU:HB3	1.76	0.66
1:A:314:VAL:H	1:A:337:ASN:ND2	1.93	0.66
1:B:164:MET:H	1:B:219:ASN:HD21	1.41	0.66
1:C:12:ASP:O	1:D:403:LEU:HD13	1.96	0.65
1:C:353:LEU:HD22	1:C:387:LEU:HD21	1.78	0.64
1:B:141:GLU:O	1:B:388:CYS:SG	2.56	0.64
1:B:314:VAL:H	1:B:337:ASN:HD21	1.44	0.63
1:B:196:LYS:HE3	1:B:201:LYS:CG	2.28	0.63
1:D:142:VAL:HG13	1:D:385:VAL:CG1	2.29	0.63
1:D:164:MET:H	1:D:219:ASN:HD21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG22	1:B:128:PRO:HD2	1.81	0.62
1:C:196:LYS:HE3	1:C:201:LYS:CG	2.25	0.62
1:D:127:VAL:CG2	1:D:131:ARG:HG2	2.29	0.62
1:C:314:VAL:N	1:C:337:ASN:HD21	1.97	0.62
1:B:314:VAL:H	1:B:337:ASN:ND2	1.98	0.62
1:B:176:ASN:C	1:B:176:ASN:HD22	2.09	0.61
1:B:53:LYS:HD2	4:B:585:HOH:O	2.00	0.61
1:B:322:THR:HG23	1:B:341:LEU:HD12	1.83	0.61
1:C:82:ASN:ND2	1:C:84:THR:OG1	2.33	0.61
1:B:337:ASN:C	1:B:337:ASN:HD22	2.08	0.61
1:A:350:THR:O	1:A:354:GLN:HG3	2.01	0.60
1:C:150:ASN:CG	1:C:166:GLU:HB3	2.26	0.60
1:C:176:ASN:ND2	1:C:179:GLU:H	1.99	0.60
1:A:403:LEU:HD13	1:B:12:ASP:O	2.01	0.60
1:D:328:ALA:O	1:D:331:VAL:HG22	2.01	0.60
1:C:9:GLU:HG3	1:C:61:VAL:HG23	1.82	0.60
1:A:30:PHE:HE1	1:A:123:VAL:HG21	1.66	0.60
1:C:81:LEU:HD11	1:C:92:LEU:HD12	1.84	0.60
1:C:265:ASP:O	1:C:268:ARG:HG2	2.01	0.59
1:C:143:ILE:C	1:C:143:ILE:HD12	2.27	0.59
1:D:127:VAL:HG22	1:D:128:PRO:HD2	1.85	0.59
1:A:337:ASN:C	1:A:337:ASN:HD22	2.11	0.58
1:A:12:ASP:O	1:B:403:LEU:HD13	2.03	0.58
1:B:142:VAL:HG13	1:B:385:VAL:HG12	1.85	0.58
1:D:337:ASN:C	1:D:337:ASN:HD22	2.12	0.58
1:B:328:ALA:O	1:B:331:VAL:HG22	2.04	0.58
1:D:164:MET:HG3	1:D:219:ASN:ND2	2.19	0.57
1:C:127:VAL:CG2	1:C:131:ARG:HG2	2.35	0.56
1:A:370:HIS:CD2	1:A:370:HIS:H	2.24	0.56
1:D:97:ASP:OD2	1:D:102:LYS:HA	2.06	0.56
1:D:143:ILE:HD11	1:D:390:GLY:HA2	1.86	0.56
1:B:244:ASP:HA	1:B:292:GLU:HB3	1.88	0.56
1:B:313:GLN:HA	1:B:337:ASN:HD21	1.70	0.56
1:C:275:LEU:HG	1:C:279:TYR:CE2	2.40	0.56
1:C:340:LEU:CD2	1:C:342:LYS:HE3	2.35	0.55
1:A:127:VAL:HG22	1:A:128:PRO:HD2	1.88	0.55
1:D:143:ILE:HD12	1:D:144:LEU:O	2.06	0.55
1:C:176:ASN:ND2	1:C:178:ARG:HG3	2.20	0.55
1:D:143:ILE:HD13	1:D:423:ALA:HB2	1.89	0.55
1:C:164:MET:H	1:C:219:ASN:HD21	1.54	0.54
1:C:328:ALA:O	1:C:331:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LYS:NZ	1:C:201:LYS:HE2	2.23	0.54
1:A:176:ASN:ND2	1:A:179:GLU:H	2.05	0.53
1:B:142:VAL:HG13	1:B:385:VAL:HG13	1.89	0.53
1:A:164:MET:H	1:A:219:ASN:HD21	1.56	0.53
1:C:9:GLU:HG3	1:C:61:VAL:CG2	2.39	0.53
1:C:327:ILE:O	1:C:331:VAL:HG13	2.09	0.53
1:C:337:ASN:C	1:C:337:ASN:HD22	2.17	0.53
1:A:331:VAL:HG23	1:A:332:ASN:N	2.24	0.53
1:B:196:LYS:HE3	1:B:201:LYS:HG2	1.91	0.53
1:B:353:LEU:O	1:B:357:LYS:HG2	2.09	0.53
1:B:398:CYS:O	1:B:399:ARG:HB2	2.09	0.53
1:D:23:LEU:HD23	1:D:23:LEU:C	2.34	0.52
1:A:75:ALA:O	1:A:79:LYS:HG2	2.09	0.52
1:C:82:ASN:ND2	1:C:84:THR:H	2.06	0.52
1:B:43:TYR:OH	1:B:298:ASP:OD2	2.26	0.52
1:A:141:GLU:O	1:A:388:CYS:SG	2.68	0.52
1:C:150:ASN:ND2	1:C:166:GLU:HB3	2.25	0.52
1:C:161:LYS:HB3	1:C:217:LEU:HD13	1.92	0.52
1:C:127:VAL:HG22	1:C:131:ARG:HG2	1.92	0.51
1:D:43:TYR:CE1	1:D:298:ASP:OD2	2.63	0.51
1:B:127:VAL:HG22	1:B:128:PRO:CD	2.41	0.51
1:D:164:MET:HG3	1:D:219:ASN:CG	2.35	0.51
1:B:370:HIS:CD2	1:B:370:HIS:H	2.28	0.51
1:B:125:LYS:HE2	1:B:132:HIS:ND1	2.26	0.51
1:D:82:ASN:HD21	1:D:84:THR:HG23	1.75	0.51
1:B:166:GLU:HB2	1:B:244:ASP:HB3	1.93	0.50
1:A:43:TYR:HE1	1:A:298:ASP:OD2	1.95	0.50
1:A:398:CYS:O	1:A:399:ARG:HB2	2.11	0.50
1:D:43:TYR:HE1	1:D:298:ASP:OD2	1.93	0.50
1:A:220:LYS:HE3	4:A:532:HOH:O	2.11	0.50
1:C:398:CYS:O	1:C:399:ARG:HB2	2.11	0.50
1:A:143:ILE:HD11	1:A:390:GLY:HA2	1.94	0.50
1:B:431:LEU:O	1:B:432:ALA:C	2.54	0.50
1:A:176:ASN:ND2	1:A:178:ARG:HG3	2.27	0.50
1:B:331:VAL:HG23	1:B:332:ASN:N	2.26	0.50
1:B:127:VAL:HG21	1:B:131:ARG:HG2	1.94	0.49
1:B:127:VAL:CG2	1:B:131:ARG:HG2	2.42	0.49
1:D:143:ILE:HD12	1:D:143:ILE:C	2.37	0.49
1:B:164:MET:HB2	1:B:219:ASN:ND2	2.27	0.49
1:C:164:MET:HB2	1:C:219:ASN:ND2	2.27	0.49
1:C:340:LEU:HD21	1:C:342:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASN:C	1:C:176:ASN:HD22	2.19	0.49
1:D:265:ASP:O	1:D:268:ARG:HG2	2.13	0.49
1:D:322:THR:HG23	1:D:341:LEU:HD12	1.93	0.49
1:D:313:GLN:HA	1:D:337:ASN:HD21	1.78	0.49
1:D:82:ASN:ND2	1:D:84:THR:HG23	2.28	0.49
1:B:87:GLU:O	1:B:91:LYS:HG3	2.12	0.48
1:D:266:PRO:HA	1:D:269:TYR:CE1	2.48	0.48
1:C:176:ASN:HD22	1:C:179:GLU:H	1.61	0.48
1:A:42:ILE:HG12	1:A:297:GLN:CD	2.39	0.48
1:A:244:ASP:HA	1:A:292:GLU:HB3	1.96	0.48
1:A:401:GLU:HB3	1:B:400:SER:HB2	1.96	0.48
1:B:176:ASN:HD21	1:B:179:GLU:H	1.61	0.48
1:D:314:VAL:N	1:D:337:ASN:HD21	2.05	0.48
1:D:370:HIS:CD2	1:D:370:HIS:H	2.32	0.48
1:A:150:ASN:O	1:A:396:ALA:HB2	2.13	0.48
1:D:127:VAL:HG21	1:D:131:ARG:CG	2.41	0.48
1:D:143:ILE:CD1	1:D:423:ALA:HB2	2.44	0.48
1:D:192:LYS:HB2	1:D:212:PHE:CZ	2.49	0.48
1:C:400:SER:HB2	1:D:401:GLU:HB3	1.95	0.47
1:C:403:LEU:HD22	1:D:11:PHE:CB	2.44	0.47
1:C:401:GLU:HB3	1:D:400:SER:HB2	1.96	0.47
1:C:331:VAL:CG2	1:C:332:ASN:N	2.78	0.47
1:C:395:GLY:HA3	1:C:402:ARG:HD2	1.96	0.47
1:A:79:LYS:HG3	1:A:92:LEU:HD11	1.96	0.47
1:C:143:ILE:HD12	1:C:144:LEU:O	2.14	0.47
1:A:149:PHE:O	1:A:168:MET:HA	2.14	0.47
1:C:370:HIS:H	1:C:370:HIS:CD2	2.33	0.47
1:D:322:THR:HG22	1:D:322:THR:O	2.14	0.47
1:C:164:MET:HG2	1:C:245:VAL:HG13	1.95	0.47
1:C:350:THR:O	1:C:354:GLN:HG3	2.15	0.47
1:A:293:ASP:HA	1:A:303:TRP:CH2	2.50	0.47
1:C:331:VAL:HG23	1:C:332:ASN:N	2.29	0.46
1:D:303:TRP:CE3	1:D:319:LEU:HD22	2.50	0.46
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.81	0.46
1:B:127:VAL:HG21	1:B:131:ARG:CG	2.46	0.46
1:D:164:MET:HE1	1:D:279:TYR:HE1	1.79	0.46
1:C:340:LEU:HD23	1:C:342:LYS:HE3	1.96	0.46
1:A:43:TYR:CE1	1:A:298:ASP:OD2	2.68	0.46
1:D:82:ASN:ND2	1:D:84:THR:H	2.14	0.46
1:B:164:MET:HG2	1:B:245:VAL:HG13	1.97	0.46
1:C:97:ASP:OD2	1:C:102:LYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:O	1:A:357:LYS:HG2	2.16	0.46
1:A:97:ASP:O	1:A:104:LYS:HE2	2.16	0.46
1:C:29:LEU:HD12	1:C:30:PHE:N	2.31	0.46
1:C:293:ASP:OD2	1:C:317:ASP:HB3	2.16	0.46
1:D:162:LEU:HD21	1:D:167:PHE:CE1	2.51	0.46
1:C:143:ILE:HD12	1:C:144:LEU:C	2.41	0.45
1:C:403:LEU:HD22	1:D:11:PHE:HB2	1.98	0.45
1:A:322:THR:HG23	1:A:341:LEU:HD12	1.97	0.45
1:D:142:VAL:HG13	1:D:385:VAL:HG13	1.97	0.45
1:A:11:PHE:HB2	1:B:403:LEU:HD22	1.98	0.45
1:C:245:VAL:HG11	1:C:279:TYR:OH	2.16	0.45
1:C:250:PHE:HB3	1:C:260:PHE:CD1	2.50	0.45
1:B:23:LEU:C	1:B:23:LEU:HD23	2.42	0.45
1:B:293:ASP:HA	1:B:303:TRP:CH2	2.51	0.45
1:C:14:ARG:HH12	1:C:372:SER:CB	2.29	0.45
1:D:294:PRO:HD2	1:D:303:TRP:CH2	2.51	0.45
1:A:176:ASN:C	1:A:176:ASN:HD22	2.24	0.45
1:C:11:PHE:HB2	1:D:403:LEU:HD22	1.98	0.45
1:C:142:VAL:HG22	1:C:385:VAL:HG12	1.97	0.45
1:C:224:GLU:O	1:C:228:THR:HG23	2.17	0.45
1:A:23:LEU:HD23	1:A:23:LEU:C	2.42	0.45
1:B:149:PHE:O	1:B:168:MET:HA	2.16	0.45
1:D:142:VAL:HG13	1:D:385:VAL:HG12	1.99	0.45
1:D:81:LEU:CD1	1:D:92:LEU:HD12	2.48	0.44
1:A:127:VAL:HG22	1:A:128:PRO:CD	2.47	0.44
1:A:401:GLU:HB3	1:B:400:SER:CB	2.47	0.44
1:C:43:TYR:OH	1:C:298:ASP:OD2	2.31	0.44
1:A:314:VAL:N	1:A:337:ASN:HD21	2.09	0.44
1:B:80:LYS:NZ	4:B:440:HOH:O	2.48	0.44
1:B:143:ILE:HD12	1:B:143:ILE:C	2.43	0.44
1:C:143:ILE:HD13	1:C:423:ALA:HB2	1.98	0.44
1:C:401:GLU:HB3	1:D:400:SER:CB	2.48	0.44
1:D:176:ASN:HD22	1:D:179:GLU:H	1.61	0.44
1:C:244:ASP:HA	1:C:292:GLU:HB3	2.00	0.43
1:D:143:ILE:HD12	1:D:144:LEU:C	2.42	0.43
1:D:221:GLU:HA	1:D:221:GLU:OE1	2.18	0.43
1:C:322:THR:O	1:C:322:THR:HG22	2.18	0.43
1:B:157:HIS:CE1	1:B:372:SER:HB3	2.53	0.43
1:A:7:ALA:HB2	1:A:68:ILE:HG21	2.00	0.43
1:A:11:PHE:CB	1:B:403:LEU:HD22	2.48	0.43
1:B:176:ASN:HD22	1:B:179:GLU:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:O	1:B:133:ILE:HG12	2.19	0.43
1:A:250:PHE:HB3	1:A:260:PHE:CD1	2.54	0.43
1:B:328:ALA:O	1:B:331:VAL:CG2	2.66	0.43
1:A:108:ASN:OD1	1:A:108:ASN:N	2.51	0.43
1:A:127:VAL:HG21	1:A:131:ARG:HG2	2.01	0.43
1:A:315:VAL:HG22	1:A:338:CYS:HB3	2.01	0.43
1:C:161:LYS:O	1:C:162:LEU:C	2.62	0.43
1:A:143:ILE:C	1:A:143:ILE:HD12	2.44	0.43
1:D:226:LEU:O	1:D:230:ILE:HG13	2.19	0.43
1:C:370:HIS:CG	1:C:394:THR:HA	2.53	0.42
1:D:81:LEU:HD11	1:D:92:LEU:HD12	2.01	0.42
1:D:150:ASN:O	1:D:396:ALA:HB2	2.19	0.42
1:B:294:PRO:HD2	1:B:303:TRP:CH2	2.54	0.42
1:C:196:LYS:CE	1:C:201:LYS:HG2	2.35	0.42
1:A:87:GLU:HG3	1:A:350:THR:HG21	2.01	0.42
1:B:29:LEU:HD12	1:B:30:PHE:N	2.33	0.42
1:C:293:ASP:HA	1:C:303:TRP:CH2	2.54	0.42
1:B:75:ALA:O	1:B:79:LYS:HG2	2.18	0.42
1:B:43:TYR:CE1	1:B:298:ASP:OD2	2.73	0.42
1:D:25:THR:C	1:D:27:LYS:N	2.77	0.42
1:A:142:VAL:HG22	1:A:385:VAL:HG12	2.01	0.42
1:A:170:LEU:N	1:A:170:LEU:HD12	2.34	0.42
1:C:196:LYS:HZ1	1:C:201:LYS:HE2	1.84	0.42
1:B:192:LYS:HB2	1:B:212:PHE:CZ	2.55	0.42
1:D:169:ILE:C	1:D:170:LEU:HD12	2.44	0.42
1:D:157:HIS:CE1	1:D:372:SER:HB3	2.55	0.42
1:D:293:ASP:HA	1:D:303:TRP:CH2	2.54	0.42
1:D:398:CYS:O	1:D:399:ARG:HB2	2.19	0.42
1:A:429:ASN:HD21	1:A:431:LEU:HB2	1.85	0.42
1:D:321:VAL:HG23	1:D:323:ASN:HB2	2.01	0.42
1:B:220:LYS:HE2	1:B:286:TYR:OH	2.19	0.41
1:D:224:GLU:O	1:D:228:THR:CG2	2.68	0.41
1:C:127:VAL:HG21	1:C:131:ARG:HG2	2.02	0.41
1:D:170:LEU:HD12	1:D:170:LEU:N	2.35	0.41
1:A:401:GLU:HB3	1:B:400:SER:OG	2.19	0.41
1:C:143:ILE:CD1	1:C:423:ALA:HB2	2.49	0.41
1:C:271:SER:OG	1:C:274:GLN:HG3	2.20	0.41
1:D:161:LYS:O	1:D:162:LEU:C	2.63	0.41
1:B:119:LYS:HE2	4:B:600:HOH:O	2.20	0.41
1:B:419:LYS:HA	1:B:419:LYS:HD3	1.83	0.41
1:D:303:TRP:CD2	1:D:319:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ASN:OD1	1:D:108:ASN:N	2.49	0.41
1:A:127:VAL:CG2	1:A:131:ARG:HG2	2.51	0.41
1:A:202:ASP:OD1	1:B:160:ASN:HA	2.21	0.41
1:C:400:SER:CB	1:D:401:GLU:HB3	2.51	0.41
1:A:90:ASP:O	1:A:94:ILE:HG13	2.20	0.41
1:A:403:LEU:HD22	1:B:11:PHE:HB2	2.02	0.41
1:A:429:ASN:C	1:A:431:LEU:H	2.29	0.41
1:D:43:TYR:HD1	4:D:468:HOH:O	2.03	0.41
1:D:271:SER:HB2	1:D:272:PRO:HD2	2.02	0.41
1:D:149:PHE:O	1:D:168:MET:HA	2.21	0.41
1:A:82:ASN:ND2	1:A:84:THR:OG1	2.51	0.40
1:D:293:ASP:OD2	1:D:317:ASP:HB3	2.21	0.40
1:A:176:ASN:HD22	1:A:179:GLU:H	1.69	0.40
1:C:149:PHE:O	1:C:168:MET:HA	2.21	0.40
1:C:169:ILE:O	1:C:169:ILE:HG13	2.21	0.40
1:B:73:ALA:HB3	1:B:74:PRO:CD	2.51	0.40
1:C:35:PRO:HB2	1:C:371:ARG:HB2	2.03	0.40
1:C:143:ILE:HD11	1:C:390:GLY:HA2	2.04	0.40
1:D:70:LYS:O	1:D:74:PRO:HG3	2.22	0.40
1:C:14:ARG:HH12	1:C:372:SER:HB2	1.86	0.40
1:D:127:VAL:HG22	1:D:128:PRO:CD	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	430/433 (99%)	411 (96%)	17 (4%)	2 (0%)	24	27
1	B	430/433 (99%)	414 (96%)	16 (4%)	0	100	100
1	C	431/433 (100%)	413 (96%)	16 (4%)	2 (0%)	24	27
1	D	429/433 (99%)	412 (96%)	16 (4%)	1 (0%)	43	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1720/1732 (99%)	1650 (96%)	65 (4%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	264	ASP
1	C	264	ASP
1	A	431	LEU
1	A	399	ARG
1	C	399	ARG

5.3.2 Protein sidechains ⓘ

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	351/352 (100%)	346 (99%)	5 (1%)	59	75
1	B	351/352 (100%)	344 (98%)	7 (2%)	48	64
1	C	352/352 (100%)	341 (97%)	11 (3%)	35	48
1	D	351/352 (100%)	346 (99%)	5 (1%)	59	75
All	All	1405/1408 (100%)	1377 (98%)	28 (2%)	48	64

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	142	VAL
1	A	176	ASN
1	A	337	ASN
1	A	344	ASN
1	B	29	LEU
1	B	92	LEU
1	B	142	VAL
1	B	145	PRO
1	B	176	ASN

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Mol	Chain	Res	Type
1	B	337	ASN
1	B	344	ASN
1	C	57	MET
1	C	92	LEU
1	C	127	VAL
1	C	142	VAL
1	C	143	ILE
1	C	166	GLU
1	C	176	ASN
1	C	178	ARG
1	C	228	THR
1	C	337	ASN
1	C	344	ASN
1	D	142	VAL
1	D	143	ILE
1	D	176	ASN
1	D	228	THR
1	D	337	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	51	ASN
1	A	82	ASN
1	A	139	ASN
1	A	150	ASN
1	A	153	ASN
1	A	176	ASN
1	A	219	ASN
1	A	332	ASN
1	A	337	ASN
1	A	360	GLN
1	A	429	ASN
1	B	82	ASN
1	B	139	ASN
1	B	153	ASN
1	B	176	ASN
1	B	219	ASN
1	B	337	ASN
1	B	360	GLN
1	C	16	ASN

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Mol	Chain	Res	Type
1	C	82	ASN
1	C	139	ASN
1	C	153	ASN
1	C	176	ASN
1	C	190	ASN
1	C	219	ASN
1	C	337	ASN
1	C	360	GLN
1	D	16	ASN
1	D	82	ASN
1	D	139	ASN
1	D	153	ASN
1	D	176	ASN
1	D	219	ASN
1	D	313	GLN
1	D	332	ASN
1	D	337	ASN
1	D	360	GLN
1	D	391	GLN
1	D	429	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
3	SO4	C	436	2	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	B	436	2	4,4,4	0.45	0	6,6,6	0.16	0
3	SO4	D	436	2	4,4,4	0.36	0	6,6,6	0.42	0
3	SO4	A	436	2	4,4,4	0.46	0	6,6,6	0.34	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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/433 (99%)	-0.56	11 (2%) 58 55	8, 16, 34, 67	0
1	B	432/433 (99%)	-0.46	6 (1%) 73 71	12, 20, 35, 63	0
1	C	433/433 (100%)	-0.33	5 (1%) 76 74	11, 22, 41, 52	0
1	D	431/433 (99%)	-0.01	6 (1%) 73 71	15, 26, 44, 64	0
All	All	1728/1732 (99%)	-0.34	28 (1%) 70 67	8, 21, 40, 67	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	LEU	6.7
1	A	431	LEU	6.2
1	A	432	ALA	5.9
1	B	432	ALA	4.9
1	B	431	LEU	3.7
1	A	419	LYS	3.2
1	A	418	SER	2.9
1	B	419	LYS	2.6
1	C	201	LYS	2.6
1	C	78	SER	2.6
1	B	78	SER	2.5
1	D	197	GLU	2.4
1	D	331	VAL	2.3
1	C	178	ARG	2.3
1	A	80	LYS	2.3
1	D	70	LYS	2.3
1	A	57	MET	2.2
1	A	1	SER	2.2
1	B	178	ARG	2.1
1	A	429	ASN	2.1
1	A	81	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	429	ASN	2.1
1	A	310	ALA	2.1
1	D	269	TYR	2.0
1	C	1	SER	2.0
1	A	70	LYS	2.0
1	C	80	LYS	2.0
1	D	419	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	C	434	1/1	0.78	0.18	29,29,29,29	0
2	MG	B	435	1/1	0.86	0.15	23,23,23,23	0
2	MG	D	434	1/1	0.88	0.15	32,32,32,32	0
2	MG	A	434	1/1	0.90	0.12	18,18,18,18	0
2	MG	C	435	1/1	0.91	0.16	26,26,26,26	0
2	MG	A	435	1/1	0.92	0.16	19,19,19,19	0
2	MG	B	434	1/1	0.92	0.13	22,22,22,22	0
2	MG	D	435	1/1	0.92	0.14	30,30,30,30	0
3	SO4	D	436	5/5	0.98	0.06	18,20,23,25	0
3	SO4	B	436	5/5	0.99	0.06	15,15,17,17	0
3	SO4	C	436	5/5	0.99	0.05	12,15,18,18	0
3	SO4	A	436	5/5	0.99	0.05	9,10,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.