



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:18 AM UTC

PDB ID : 3PII / pdb_00003pii
Title : Crystal structure of Mutant of ht- Alcohol Dehydrogenase with substrate analogue butyramide
Authors : Dong, M.; Bahnson, B.J.
Deposited on : 2010-11-06
Resolution : 2.90 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

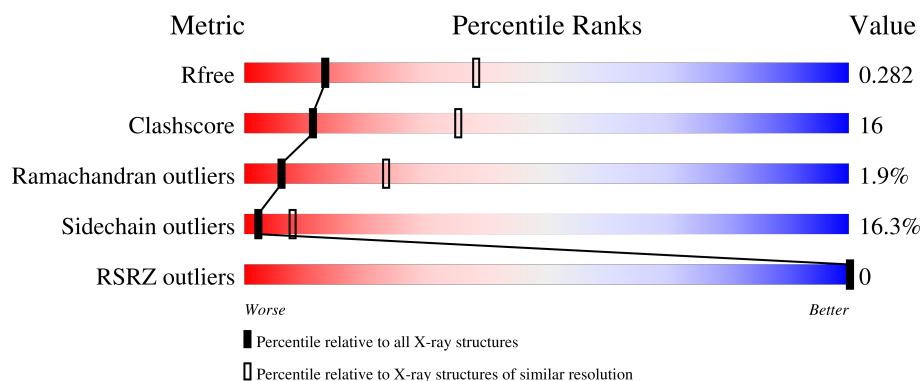
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	339	 61% 33% 5% ..
1	B	339	 67% 27%
1	C	339	 60% 32% 6% ..
1	D	339	 66% 26% 6% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10211 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 Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2539	1630	427	468	14			
1	C	337	Total	C	N	O	S	0	0	0
			2539	1630	427	468	14			
1	B	337	Total	C	N	O	S	0	0	0
			2539	1630	427	468	14			
1	D	337	Total	C	N	O	S	0	0	0
			2539	1630	427	468	14			

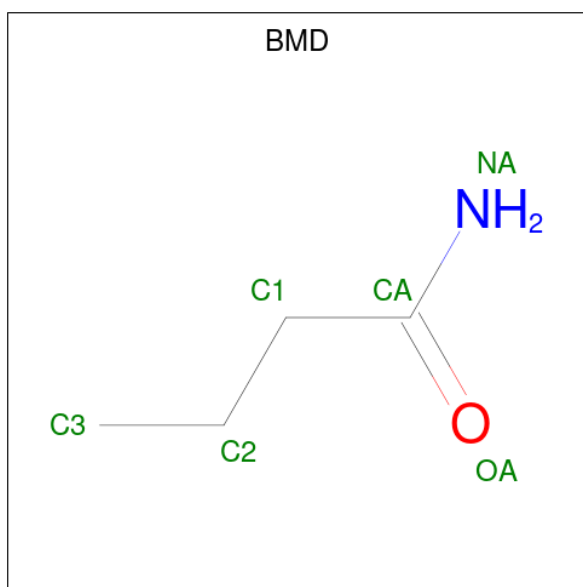
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	PHE	LEU	engineered mutation	UNP P42328
C	176	PHE	LEU	engineered mutation	UNP P42328
B	176	PHE	LEU	engineered mutation	UNP P42328
D	176	PHE	LEU	engineered mutation	UNP P42328

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

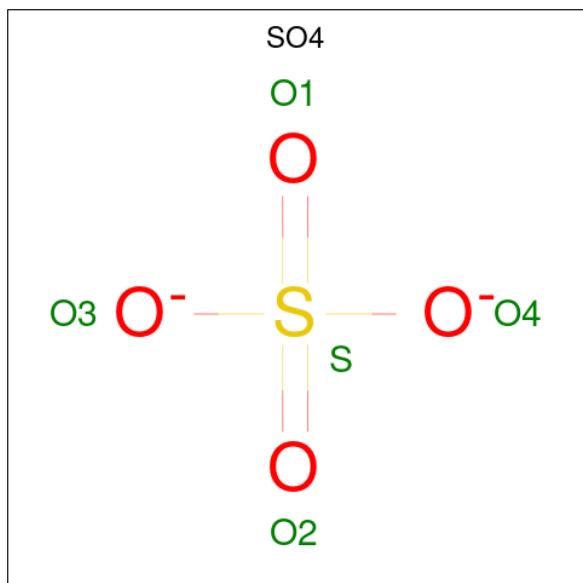
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is BUTYRAMIDE (CCD ID: BMD) (formula: C₄H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	4	1	1		
3	C	1	Total	C	N	O	0	0
			6	4	1	1		
3	B	1	Total	C	N	O	0	0
			6	4	1	1		
3	D	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

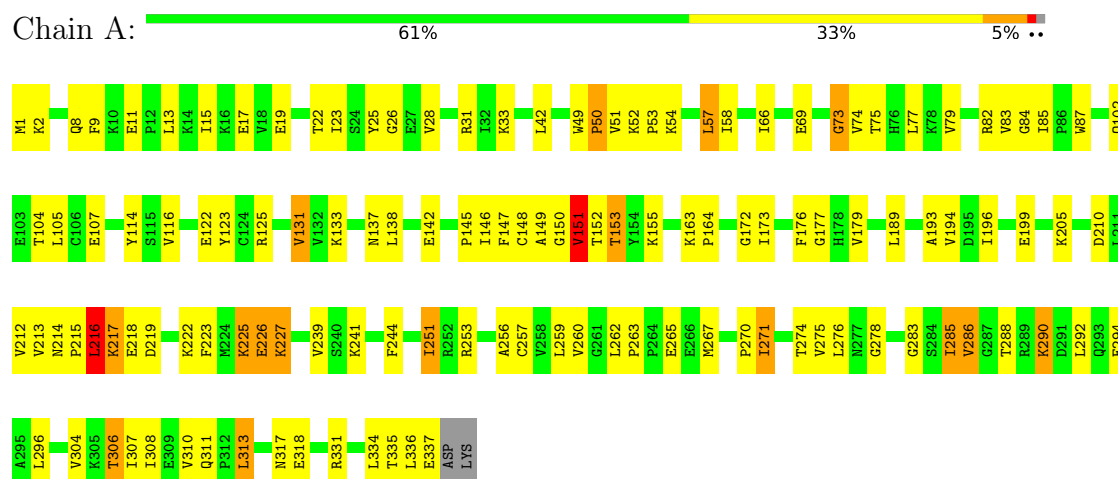
- Molecule 5 is water.

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

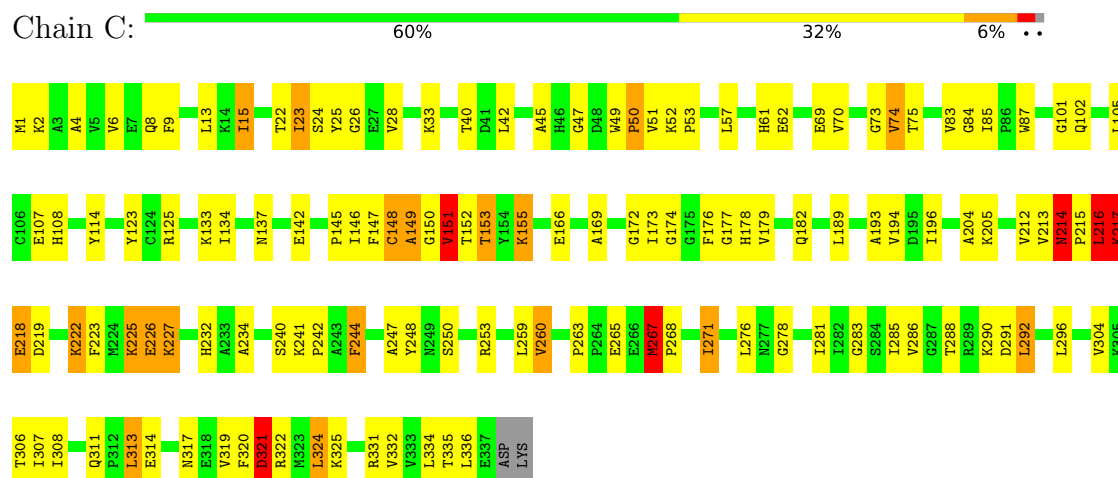
3 Residue-property plots

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: Alcohol dehydrogenase

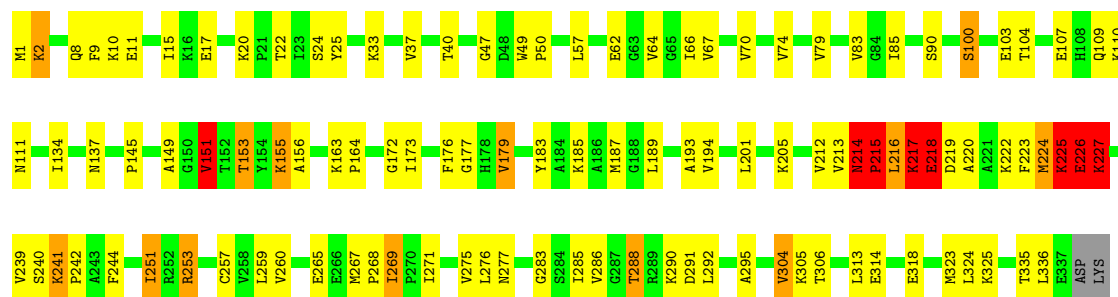


• Molecule 1: Alcohol dehydrogenase



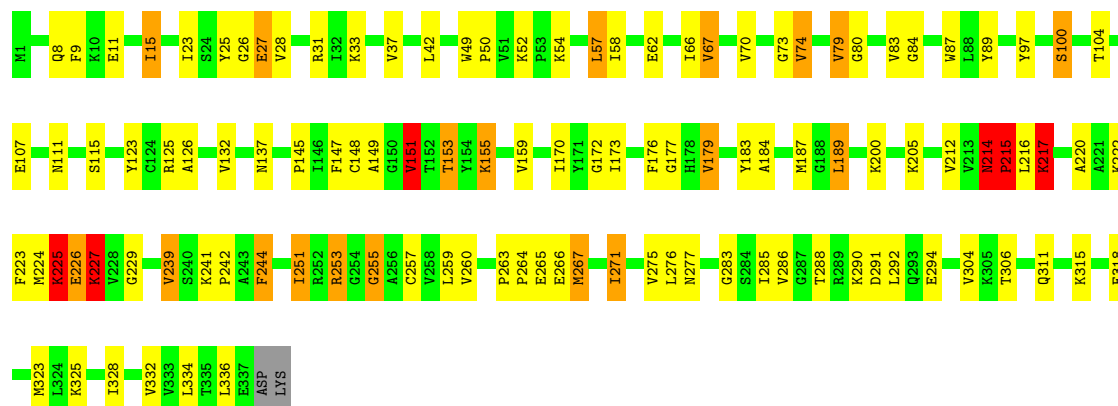
• Molecule 1: Alcohol dehydrogenase





• Molecule 1: Alcohol dehydrogenase

Chain D: 66% 26% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	145.65Å 145.65Å 135.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.61 – 2.90 49.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.61-2.90) 99.8 (49.61-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.286 0.204 , 0.282	Depositor DCC
R_{free} test set	1799 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMD, ZN, 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	0.90	2/2591 (0.1%)	1.15	11/3513 (0.3%)
1	B	0.89	3/2591 (0.1%)	1.14	14/3513 (0.4%)
1	C	0.93	2/2591 (0.1%)	1.20	20/3513 (0.6%)
1	D	0.88	0/2591	1.09	8/3513 (0.2%)
All	All	0.90	7/10364 (0.1%)	1.14	53/14052 (0.4%)

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	1
1	B	0	8
1	C	0	5
1	D	0	4
All	All	0	18

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	ILE	CA-CB	7.23	1.61	1.53
1	C	307	ILE	CA-CB	6.59	1.61	1.53
1	B	304	VAL	CA-CB	5.33	1.61	1.54
1	A	51	VAL	CA-CB	5.19	1.59	1.53
1	B	179	VAL	CA-CB	5.09	1.60	1.54
1	C	51	VAL	CA-CB	5.05	1.60	1.54
1	B	239	VAL	CA-CB	5.01	1.58	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	ASP	N-CA-C	10.00	126.47	113.18
1	D	226	GLU	CA-C-N	8.30	136.64	121.70
1	D	226	GLU	C-N-CA	8.30	136.64	121.70
1	A	216	LEU	N-CA-C	7.98	123.41	111.04
1	D	214	ASN	N-CA-C	7.71	126.85	109.81
1	C	216	LEU	N-CA-C	7.69	119.56	111.03
1	D	215	PRO	N-CA-C	-7.51	97.01	112.47
1	C	151	VAL	CB-CA-C	-7.42	102.48	111.97
1	B	214	ASN	CA-C-N	7.06	128.66	119.84
1	B	214	ASN	C-N-CA	7.06	128.66	119.84
1	A	226	GLU	CA-C-N	7.04	134.36	121.70
1	A	226	GLU	C-N-CA	7.04	134.36	121.70
1	C	226	GLU	CA-C-N	6.96	134.23	121.70
1	C	226	GLU	C-N-CA	6.96	134.23	121.70
1	C	85	ILE	CA-C-N	6.76	127.22	120.52
1	C	85	ILE	C-N-CA	6.76	127.22	120.52
1	C	215	PRO	N-CA-C	-6.75	98.55	112.47
1	C	260	VAL	CB-CA-C	6.72	117.23	110.65
1	A	151	VAL	CB-CA-C	-6.52	103.62	111.97
1	B	111	ASN	N-CA-C	6.39	118.93	108.52
1	B	218	GLU	CA-C-N	6.32	133.60	121.54
1	B	218	GLU	C-N-CA	6.32	133.60	121.54
1	B	226	GLU	N-CA-C	-6.27	105.67	113.38
1	C	73	GLY	N-CA-C	6.16	123.54	115.47
1	C	149	ALA	N-CA-C	-6.14	105.91	113.41
1	C	321	ASP	CA-C-N	6.07	132.63	121.70
1	C	321	ASP	C-N-CA	6.07	132.63	121.70
1	A	216	LEU	CA-C-N	5.76	132.06	121.70
1	A	216	LEU	C-N-CA	5.76	132.06	121.70
1	B	151	VAL	CB-CA-C	-5.70	104.57	112.04
1	C	267	MET	CA-C-N	5.69	140.66	127.00
1	C	267	MET	C-N-CA	5.69	140.66	127.00
1	C	151	VAL	N-CA-CB	5.66	117.18	110.55
1	B	225	LYS	CB-CA-C	5.63	121.62	110.42
1	D	23	ILE	N-CA-C	5.61	116.56	108.48
1	D	111	ASN	N-CA-C	5.50	118.21	109.24
1	A	73	GLY	N-CA-C	5.48	122.38	115.42
1	B	85	ILE	CA-C-N	5.43	125.42	120.21
1	B	85	ILE	C-N-CA	5.43	125.42	120.21
1	C	214	ASN	N-CA-C	5.41	120.75	108.74
1	B	240	SER	N-CA-C	-5.39	101.78	110.14
1	A	66	ILE	N-CA-C	5.34	116.17	108.48
1	D	151	VAL	CB-CA-C	-5.24	105.17	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ASP	N-CA-CB	5.19	119.26	110.49
1	B	295	ALA	N-CA-C	-5.16	105.66	111.28
1	D	255	GLY	N-CA-C	5.15	119.14	112.54
1	B	66	ILE	CB-CA-C	-5.15	102.98	110.81
1	A	210	ASP	N-CA-C	5.11	116.92	111.36
1	C	23	ILE	N-CA-C	5.09	115.30	107.77
1	C	134	ILE	N-CA-C	-5.07	104.27	108.63
1	A	85	ILE	CA-C-N	5.05	126.38	120.98
1	A	85	ILE	C-N-CA	5.05	126.38	120.98
1	C	218	GLU	N-CA-C	5.05	117.98	108.65

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	LYS	Peptide
1	B	214	ASN	Peptide
1	B	215	PRO	Peptide
1	B	217	LYS	Peptide
1	B	218	GLU	Peptide
1	B	224	MET	Peptide
1	B	225	LYS	Peptide
1	B	226	GLU	Mainchain,Peptide
1	C	148	CYS	Peptide
1	C	214	ASN	Peptide
1	C	217	LYS	Peptide
1	C	225	LYS	Peptide
1	C	321	ASP	Peptide
1	D	214	ASN	Peptide
1	D	215	PRO	Peptide
1	D	217	LYS	Peptide
1	D	225	LYS	Peptide

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	2539	0	2586	84	0
1	B	2539	0	2586	99	0
1	C	2539	0	2586	94	0
1	D	2539	0	2586	85	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	6	0	9	2	0
3	B	6	0	9	3	0
3	C	6	0	9	0	0
3	D	6	0	9	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	10211	0	10380	334	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 16.

All (334) 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:B:215:PRO:HD2	1:B:216:LEU:CD2	1.56	1.34
1:B:215:PRO:CD	1:B:216:LEU:HD22	1.54	1.33
1:B:214:ASN:OD1	1:B:216:LEU:HD21	1.16	1.29
1:B:226:GLU:H	1:B:227:LYS:CB	1.48	1.26
1:B:215:PRO:CD	1:B:216:LEU:CD2	2.11	1.20
1:C:216:LEU:CB	1:C:217:LYS:HB2	1.69	1.19
1:B:216:LEU:O	1:B:217:LYS:HG2	1.39	1.18
1:D:239:VAL:HG12	1:D:267:MET:CE	1.77	1.14
1:B:214:ASN:OD1	1:B:216:LEU:CD2	1.98	1.10
1:C:216:LEU:HB3	1:C:217:LYS:HB2	1.19	1.08
1:D:288:THR:HG22	1:D:290:LYS:H	1.14	1.08
1:B:216:LEU:O	1:B:216:LEU:HD23	1.55	1.04
1:B:226:GLU:H	1:B:227:LYS:HB2	1.19	1.03
1:B:226:GLU:N	1:B:227:LYS:CB	2.22	1.02
1:B:223:PHE:O	1:B:227:LYS:HG2	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLU:H	1:B:227:LYS:HB3	1.22	0.99
1:B:217:LYS:O	1:B:217:LYS:HG3	1.63	0.98
1:A:196:ILE:O	1:A:214:ASN:ND2	1.98	0.96
1:D:214:ASN:O	1:D:216:LEU:HB3	1.66	0.94
1:C:216:LEU:CB	1:C:217:LYS:CB	2.46	0.94
1:B:215:PRO:N	1:B:216:LEU:HD23	1.84	0.93
1:B:216:LEU:O	1:B:217:LYS:CG	2.15	0.93
1:B:226:GLU:N	1:B:227:LYS:HB2	1.84	0.92
1:D:239:VAL:HG12	1:D:267:MET:HE2	1.54	0.89
1:D:288:THR:HG22	1:D:290:LYS:N	1.88	0.89
1:D:216:LEU:O	1:D:217:LYS:HB3	1.73	0.88
1:A:226:GLU:HB3	1:A:227:LYS:HB2	1.55	0.88
1:B:215:PRO:N	1:B:216:LEU:CD2	2.37	0.86
1:C:150:GLY:O	1:C:153:THR:HG22	1.76	0.84
1:C:288:THR:HG22	1:C:290:LYS:H	1.42	0.83
1:D:214:ASN:O	1:D:214:ASN:OD1	1.97	0.82
1:C:13:LEU:H	1:C:317:ASN:HD21	1.27	0.79
1:B:216:LEU:CD2	1:B:216:LEU:O	2.30	0.79
1:A:288:THR:HG22	1:A:290:LYS:H	1.48	0.79
1:C:263:PRO:HD2	1:B:271:ILE:HG21	1.65	0.79
1:B:223:PHE:O	1:B:227:LYS:CG	2.30	0.78
1:B:226:GLU:N	1:B:227:LYS:HB3	1.92	0.78
1:C:216:LEU:HB2	1:C:217:LYS:CB	2.12	0.78
1:B:40:THR:HG21	3:B:500:BMD:H11	1.64	0.77
1:C:263:PRO:HD2	1:B:271:ILE:CG2	2.15	0.77
1:B:288:THR:HG22	1:B:290:LYS:N	1.98	0.77
1:A:222:LYS:O	1:A:226:GLU:HB2	1.87	0.74
1:B:201:LEU:HD11	1:B:214:ASN:HB2	1.69	0.73
1:D:149:ALA:O	1:D:153:THR:HB	1.89	0.72
1:B:151:VAL:HG13	1:B:292:LEU:HA	1.72	0.72
1:C:102:GLN:HB3	1:C:105:LEU:HD12	1.72	0.72
1:C:13:LEU:N	1:C:317:ASN:HD21	1.87	0.71
1:C:244:PHE:C	1:C:244:PHE:HD1	1.98	0.71
1:B:149:ALA:O	1:B:153:THR:HB	1.91	0.71
1:B:288:THR:HG22	1:B:290:LYS:H	1.55	0.70
1:A:146:ILE:HG21	1:A:296:LEU:HD23	1.72	0.70
1:C:244:PHE:C	1:C:244:PHE:CD1	2.70	0.70
1:A:13:LEU:H	1:A:317:ASN:HD21	1.39	0.70
1:C:271:ILE:HD11	1:B:267:MET:HB2	1.74	0.69
1:B:216:LEU:HD23	1:B:216:LEU:C	2.15	0.69
1:D:239:VAL:HG12	1:D:267:MET:HE1	1.69	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:MET:HB3	1:C:268:PRO:CA	2.22	0.69
1:A:263:PRO:HD2	1:D:271:ILE:CG2	2.23	0.69
1:B:226:GLU:CA	1:B:227:LYS:HB2	2.22	0.68
1:A:193:ALA:HB3	1:A:212:VAL:HG12	1.74	0.68
1:B:214:ASN:O	1:B:217:LYS:HG2	1.94	0.68
1:D:67:VAL:HG12	1:D:79:VAL:HA	1.77	0.67
1:A:13:LEU:N	1:A:317:ASN:HD21	1.93	0.67
1:C:151:VAL:HG13	1:C:292:LEU:HD13	1.77	0.67
1:C:42:LEU:HD11	1:C:324:LEU:HD12	1.77	0.66
1:C:214:ASN:C	1:C:216:LEU:H	2.01	0.66
1:B:216:LEU:O	1:B:217:LYS:CB	2.43	0.66
1:B:2:LYS:NZ	1:B:314:GLU:OE2	2.29	0.66
1:C:216:LEU:HB2	1:C:217:LYS:HB2	1.65	0.66
1:B:214:ASN:C	1:B:216:LEU:HD23	2.20	0.66
1:A:219:ASP:OD2	1:A:222:LYS:HB2	1.96	0.65
1:D:151:VAL:HG22	1:D:292:LEU:HD13	1.77	0.65
1:D:251:ILE:HD13	1:D:257:CYS:HB2	1.79	0.65
1:A:150:GLY:O	1:A:153:THR:HG22	1.96	0.64
1:C:173:ILE:O	1:C:173:ILE:HG22	1.97	0.64
1:C:149:ALA:O	1:C:153:THR:HB	1.98	0.64
1:A:267:MET:HB3	1:D:271:ILE:HD13	1.80	0.64
1:A:153:THR:HG21	1:A:179:VAL:HG23	1.79	0.64
1:A:102:GLN:HB3	1:A:105:LEU:HD12	1.79	0.63
1:B:215:PRO:HD2	1:B:216:LEU:HD22	0.70	0.63
1:C:146:ILE:HG21	1:C:296:LEU:HD23	1.80	0.63
1:A:263:PRO:HD2	1:D:271:ILE:HG21	1.80	0.63
1:B:251:ILE:HD13	1:B:257:CYS:HB2	1.81	0.62
1:B:251:ILE:CD1	1:B:257:CYS:HB2	2.29	0.62
1:D:239:VAL:CG1	1:D:267:MET:HE2	2.29	0.62
1:C:222:LYS:O	1:C:226:GLU:HB2	1.99	0.62
1:A:142:GLU:O	1:A:145:PRO:HD2	2.00	0.62
1:A:271:ILE:CD1	1:D:267:MET:HB2	2.30	0.62
1:C:267:MET:HG2	1:B:271:ILE:HD11	1.81	0.62
1:D:62:GLU:OE1	1:D:145:PRO:HA	2.00	0.62
1:C:155:LYS:HG2	1:C:291:ASP:OD2	2.00	0.61
1:B:193:ALA:HB3	1:B:212:VAL:HG12	1.82	0.61
1:A:218:GLU:HG2	1:A:219:ASP:N	2.14	0.61
1:B:8:GLN:HB2	1:B:11:GLU:HG3	1.82	0.61
1:C:216:LEU:HB2	1:C:217:LYS:HB3	1.83	0.60
1:A:278:GLY:HA2	1:D:283:GLY:O	2.02	0.60
1:A:146:ILE:CG2	1:A:296:LEU:HD23	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:THR:CG2	1:B:290:LYS:H	2.14	0.60
1:B:244:PHE:HZ	1:B:269:ILE:HG22	1.66	0.60
1:D:244:PHE:HD1	1:D:244:PHE:C	2.09	0.60
1:A:23:ILE:HG22	1:A:125:ARG:HG3	1.84	0.59
1:A:263:PRO:HG2	1:D:271:ILE:HG21	1.83	0.59
1:C:13:LEU:H	1:C:317:ASN:ND2	2.00	0.59
1:D:216:LEU:O	1:D:217:LYS:CB	2.49	0.59
1:A:271:ILE:HD11	1:D:267:MET:HB2	1.84	0.59
1:B:37:VAL:HG12	1:B:323:MET:HE1	1.86	0.58
1:A:2:LYS:HG2	1:A:122:GLU:OE2	2.03	0.58
1:C:142:GLU:O	1:C:145:PRO:HD2	2.04	0.58
1:D:244:PHE:C	1:D:244:PHE:CD1	2.81	0.58
1:C:267:MET:HB3	1:C:268:PRO:HA	1.85	0.58
1:C:4:ALA:HB2	1:C:313:LEU:HD21	1.86	0.58
1:C:268:PRO:HA	1:B:268:PRO:HA	1.85	0.58
1:C:194:VAL:HG22	1:C:213:VAL:HG12	1.84	0.57
1:D:153:THR:HG21	1:D:179:VAL:HG23	1.86	0.57
1:D:173:ILE:O	1:D:200:LYS:HE2	2.04	0.57
1:C:319:VAL:HG11	1:C:332:VAL:HG11	1.87	0.56
1:C:172:GLY:O	1:C:177:GLY:HA3	2.04	0.56
1:C:62:GLU:OE1	1:C:145:PRO:HA	2.05	0.56
1:C:153:THR:HG21	1:C:179:VAL:HG23	1.88	0.56
1:D:155:LYS:HD2	1:D:159:VAL:HG23	1.88	0.56
1:D:15:ILE:HD12	1:D:15:ILE:H	1.69	0.56
1:B:241:LYS:HG2	1:B:242:PRO:HD3	1.87	0.56
1:D:28:VAL:HG12	1:D:70:VAL:HA	1.87	0.56
1:D:57:LEU:HD22	1:D:58:ILE:N	2.21	0.55
1:B:215:PRO:CD	1:B:216:LEU:HD21	2.29	0.55
1:C:219:ASP:CG	1:C:222:LYS:HB2	2.31	0.55
1:B:214:ASN:OD1	1:B:214:ASN:C	2.49	0.55
1:C:23:ILE:O	1:C:23:ILE:HG13	2.07	0.55
1:C:226:GLU:H	1:C:227:LYS:HB3	1.71	0.55
1:A:57:LEU:HD22	1:A:58:ILE:N	2.22	0.55
1:A:251:ILE:HD11	1:A:256:ALA:O	2.07	0.54
1:A:263:PRO:CG	1:D:271:ILE:HG21	2.37	0.54
1:B:217:LYS:C	1:B:218:GLU:O	2.50	0.54
1:C:182:GLN:CB	1:C:304:VAL:HG12	2.37	0.54
1:C:244:PHE:HD1	1:C:244:PHE:O	1.90	0.54
1:C:214:ASN:C	1:C:214:ASN:OD1	2.50	0.54
1:B:217:LYS:O	1:B:217:LYS:CG	2.42	0.54
1:A:311:GLN:O	1:A:334:LEU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:O	1:B:216:LEU:CG	2.55	0.54
1:A:244:PHE:CD1	1:A:244:PHE:C	2.87	0.53
1:B:15:ILE:H	1:B:15:ILE:HD12	1.71	0.53
1:D:244:PHE:HD1	1:D:244:PHE:O	1.90	0.53
1:A:149:ALA:HA	1:A:176:PHE:CE2	2.44	0.53
1:C:263:PRO:CD	1:B:271:ILE:HG21	2.35	0.53
1:C:226:GLU:HB3	1:C:227:LYS:HB2	1.91	0.53
1:C:149:ALA:HB1	1:C:176:PHE:CD2	2.43	0.53
1:C:288:THR:HG22	1:C:290:LYS:N	2.19	0.52
1:D:151:VAL:CG2	1:D:292:LEU:HD13	2.39	0.52
1:D:184:ALA:O	1:D:189:LEU:HB2	2.10	0.52
1:A:223:PHE:CE2	1:A:227:LYS:HE3	2.45	0.52
1:C:214:ASN:O	1:C:216:LEU:N	2.32	0.52
1:C:174:GLY:O	1:C:178:HIS:HB3	2.10	0.52
1:A:173:ILE:CD1	1:A:193:ALA:HB1	2.40	0.52
1:A:263:PRO:CD	1:D:271:ILE:HG21	2.40	0.52
1:D:251:ILE:HG23	1:D:255:GLY:HA3	1.92	0.52
1:D:226:GLU:H	1:D:227:LYS:HB3	1.75	0.52
1:A:270:PRO:O	1:A:274:THR:OG1	2.23	0.52
1:C:214:ASN:O	1:C:217:LYS:HB3	2.09	0.52
1:B:223:PHE:O	1:B:227:LYS:CB	2.58	0.52
1:A:179:VAL:HG11	1:A:306:THR:HG23	1.92	0.51
1:C:149:ALA:HB1	1:C:176:PHE:HD2	1.74	0.51
1:D:67:VAL:HG12	1:D:67:VAL:O	2.10	0.51
1:C:263:PRO:HD2	1:B:271:ILE:HG22	1.93	0.51
1:B:183:TYR:O	1:B:187:MET:HG3	2.10	0.51
1:A:1:MET:SD	1:A:123:TYR:HB2	2.50	0.51
1:A:25:TYR:CE2	1:C:25:TYR:CE2	2.99	0.51
1:B:214:ASN:O	1:B:217:LYS:CG	2.59	0.51
1:D:26:GLY:HA2	1:D:74:VAL:HG12	1.92	0.51
1:C:283:GLY:HA3	1:B:275:VAL:HA	1.92	0.51
1:D:151:VAL:HG13	1:D:292:LEU:HA	1.93	0.51
1:A:49:TRP:O	1:A:50:PRO:C	2.52	0.50
1:B:220:ALA:O	1:B:224:MET:HB2	2.11	0.50
1:A:33:LYS:HZ2	1:A:337:GLU:HG3	1.77	0.50
1:A:283:GLY:HA3	1:D:275:VAL:HA	1.92	0.50
1:A:33:LYS:NZ	1:A:337:GLU:HG3	2.27	0.50
1:A:173:ILE:HD11	1:A:193:ALA:HB1	1.93	0.50
1:C:146:ILE:CG2	1:C:296:LEU:HD23	2.42	0.50
1:C:216:LEU:CA	1:C:217:LYS:CB	2.90	0.50
1:D:172:GLY:O	1:D:177:GLY:HA3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:HG12	1:C:70:VAL:HG12	1.94	0.49
1:C:244:PHE:CE1	1:C:248:TYR:HB2	2.47	0.49
1:A:285:ILE:HG23	1:A:286:VAL:HG22	1.94	0.49
1:D:264:PRO:HG2	1:D:265:GLU:H	1.77	0.49
1:B:244:PHE:CZ	1:B:269:ILE:HG22	2.47	0.49
1:C:61:HIS:HB2	1:C:87:TRP:HA	1.94	0.49
1:C:23:ILE:HG22	1:C:125:ARG:HG3	1.94	0.49
1:C:25:TYR:CD2	1:C:26:GLY:N	2.81	0.49
1:C:182:GLN:HB2	1:C:304:VAL:HG12	1.95	0.49
1:B:62:GLU:OE1	1:B:145:PRO:HA	2.12	0.49
1:B:214:ASN:C	1:B:216:LEU:CD2	2.84	0.49
1:B:217:LYS:O	1:B:218:GLU:HG2	2.13	0.49
1:D:251:ILE:CD1	1:D:257:CYS:HB2	2.41	0.49
1:A:290:LYS:HD3	1:A:294:GLU:OE2	2.13	0.48
1:C:84:GLY:HA3	1:C:147:PHE:CE2	2.48	0.48
1:C:151:VAL:O	1:C:152:THR:C	2.55	0.48
1:D:288:THR:CG2	1:D:290:LYS:H	2.04	0.48
1:B:67:VAL:HG12	1:B:79:VAL:HA	1.96	0.48
1:D:241:LYS:HB2	1:D:242:PRO:HD3	1.94	0.48
1:D:27:GLU:OE1	1:D:125:ARG:HD2	2.13	0.48
1:A:151:VAL:O	1:A:152:THR:C	2.57	0.48
1:C:15:ILE:HG21	1:C:314:GLU:HG3	1.94	0.48
1:D:8:GLN:HB2	1:D:11:GLU:HG3	1.95	0.48
1:A:172:GLY:O	1:A:177:GLY:HA3	2.13	0.48
1:A:77:LEU:HD11	1:A:131:VAL:HG22	1.96	0.47
1:A:84:GLY:HA3	1:A:147:PHE:CE2	2.48	0.47
1:C:271:ILE:CD1	1:B:267:MET:HB2	2.42	0.47
1:C:278:GLY:HA2	1:B:283:GLY:O	2.14	0.47
1:A:313:LEU:HD22	1:A:313:LEU:O	2.15	0.47
1:C:4:ALA:HB2	1:C:313:LEU:CD2	2.44	0.47
1:D:215:PRO:HB3	1:D:220:ALA:HB2	1.97	0.47
1:D:227:LYS:HA	1:D:227:LYS:HD3	1.62	0.47
1:A:214:ASN:C	1:A:216:LEU:H	2.22	0.47
1:D:87:TRP:CE2	3:D:400:BMD:H21	2.49	0.47
1:B:225:LYS:HD3	1:B:225:LYS:HA	1.77	0.47
1:D:225:LYS:O	1:D:229:GLY:HA2	2.15	0.46
1:A:239:VAL:HB	1:A:263:PRO:HG3	1.97	0.46
1:B:214:ASN:O	1:B:216:LEU:O	2.33	0.46
1:C:166:GLU:HG2	1:C:232:HIS:CE1	2.50	0.46
1:B:40:THR:CG2	3:B:500:BMD:H11	2.38	0.46
1:C:241:LYS:H	1:C:241:LYS:HG2	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ILE:HG23	1:D:80:GLY:HA2	1.96	0.46
1:A:104:THR:HG23	1:A:105:LEU:HG	1.97	0.46
1:C:1:MET:SD	1:C:123:TYR:HB2	2.56	0.46
1:A:23:ILE:O	1:A:23:ILE:HG13	2.16	0.46
1:D:89:TYR:CE1	1:D:126:ALA:HA	2.51	0.46
1:C:173:ILE:HG12	1:C:204:ALA:HB2	1.98	0.46
1:B:151:VAL:CG1	1:B:292:LEU:HA	2.44	0.46
1:B:155:LYS:O	1:B:156:ALA:C	2.59	0.45
1:D:225:LYS:HD2	1:D:225:LYS:HA	1.77	0.45
1:D:226:GLU:H	1:D:227:LYS:CB	2.29	0.45
1:B:194:VAL:HG22	1:B:213:VAL:HG12	1.99	0.45
1:D:37:VAL:HG12	1:D:323:MET:HE1	1.98	0.45
1:A:173:ILE:O	1:A:173:ILE:HG22	2.15	0.45
1:A:214:ASN:OD1	1:A:216:LEU:N	2.49	0.45
1:D:215:PRO:HG2	1:D:216:LEU:HB2	1.99	0.45
1:A:288:THR:HG22	1:A:290:LYS:N	2.23	0.45
1:B:222:LYS:O	1:B:226:GLU:HB2	2.16	0.45
1:A:194:VAL:HG22	1:A:213:VAL:HG13	1.99	0.45
1:C:49:TRP:O	1:C:50:PRO:C	2.59	0.45
1:B:15:ILE:HD12	1:B:15:ILE:N	2.31	0.45
1:B:213:VAL:HG22	1:B:214:ASN:H	1.82	0.45
1:D:288:THR:HB	1:D:291:ASP:H	1.82	0.45
1:C:2:LYS:HE3	1:C:314:GLU:OE2	2.17	0.45
1:B:226:GLU:CB	1:B:227:LYS:HB2	2.47	0.45
1:A:84:GLY:HA3	1:A:147:PHE:CZ	2.52	0.44
1:D:311:GLN:O	1:D:334:LEU:HA	2.17	0.44
1:A:25:TYR:CD2	1:A:26:GLY:N	2.86	0.44
1:A:145:PRO:HB2	1:A:306:THR:HG21	1.99	0.44
1:B:227:LYS:HA	1:B:227:LYS:HD3	1.42	0.44
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.86	0.44
1:A:270:PRO:HA	1:D:266:GLU:HG2	1.98	0.44
1:C:173:ILE:O	1:C:173:ILE:CG2	2.66	0.44
1:C:193:ALA:HB3	1:C:212:VAL:HG12	2.00	0.44
1:C:244:PHE:CD1	1:C:244:PHE:O	2.70	0.44
1:B:201:LEU:CD1	1:B:214:ASN:HB2	2.45	0.44
1:A:148:CYS:SG	3:A:600:BMD:NA	2.82	0.44
1:A:267:MET:HB3	1:D:271:ILE:CD1	2.47	0.44
1:B:90:SER:O	1:B:109:GLN:HA	2.18	0.43
1:D:84:GLY:HA3	1:D:147:PHE:CE2	2.53	0.43
1:D:214:ASN:O	1:D:214:ASN:CG	2.57	0.43
1:A:214:ASN:HA	1:A:215:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LYS:O	1:D:226:GLU:HB2	2.18	0.43
1:D:253:ARG:HG2	1:D:277:ASN:HB3	2.00	0.43
1:C:6:VAL:HG11	1:C:45:ALA:HA	2.01	0.43
1:A:25:TYR:CZ	1:A:73:GLY:HA3	2.53	0.43
1:A:271:ILE:HD13	1:D:267:MET:HB2	1.99	0.43
1:A:310:VAL:O	1:A:311:GLN:HG2	2.19	0.43
1:B:216:LEU:CD2	1:B:216:LEU:N	2.81	0.43
1:D:223:PHE:O	1:D:227:LYS:CB	2.65	0.43
1:A:53:PRO:HD3	1:A:114:TYR:CZ	2.54	0.43
1:C:26:GLY:HA2	1:C:74:VAL:HG12	2.01	0.43
1:B:67:VAL:HG12	1:B:67:VAL:O	2.18	0.43
1:B:149:ALA:HA	1:B:176:PHE:CE2	2.54	0.43
1:B:241:LYS:HB3	1:B:267:MET:HG2	2.00	0.43
1:B:288:THR:HG22	1:B:291:ASP:H	1.84	0.43
1:C:169:ALA:O	1:C:234:ALA:HA	2.18	0.43
1:B:172:GLY:O	1:B:177:GLY:HA3	2.19	0.43
1:D:31:ARG:HB2	1:D:123:TYR:CE1	2.53	0.43
1:D:132:VAL:HG21	1:D:292:LEU:HD23	2.01	0.43
1:C:196:ILE:O	1:C:214:ASN:ND2	2.49	0.43
1:D:216:LEU:O	1:D:216:LEU:HG	2.18	0.43
1:A:241:LYS:HE2	1:A:265:GLU:HG3	2.01	0.43
1:C:70:VAL:HB	1:C:74:VAL:CG2	2.49	0.43
1:B:244:PHE:CD1	1:B:244:PHE:C	2.97	0.43
1:A:149:ALA:O	1:A:153:THR:HB	2.18	0.42
1:C:223:PHE:O	1:C:227:LYS:HB3	2.19	0.42
1:C:311:GLN:O	1:C:334:LEU:HA	2.19	0.42
1:D:224:MET:O	1:D:225:LYS:C	2.60	0.42
1:A:9:PHE:C	1:A:11:GLU:H	2.27	0.42
1:A:82:ARG:NH2	1:A:138:LEU:O	2.42	0.42
1:A:275:VAL:HA	1:D:283:GLY:HA3	2.01	0.42
1:C:226:GLU:H	1:C:227:LYS:CB	2.32	0.42
1:C:240:SER:OG	1:C:242:PRO:HD2	2.20	0.42
1:B:253:ARG:HG2	1:B:277:ASN:HB3	2.00	0.42
1:A:87:TRP:CZ2	3:A:600:BMD:H32	2.55	0.42
1:A:216:LEU:CB	1:A:217:LYS:HB3	2.50	0.42
1:B:213:VAL:HG22	1:B:214:ASN:N	2.34	0.42
1:A:262:LEU:N	1:A:263:PRO:HD3	2.34	0.42
1:C:223:PHE:O	1:C:227:LYS:CB	2.67	0.42
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.88	0.42
1:B:40:THR:HG21	3:B:500:BMD:C1	2.42	0.41
1:A:271:ILE:CG2	1:D:263:PRO:HD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:MET:CB	1:D:271:ILE:HD13	2.47	0.41
1:A:223:PHE:O	1:A:226:GLU:HB3	2.21	0.41
1:B:9:PHE:CD1	1:B:47:GLY:HA3	2.56	0.41
1:D:25:TYR:CE2	1:D:73:GLY:HA3	2.56	0.41
1:A:214:ASN:OD1	1:A:216:LEU:HB2	2.21	0.41
1:D:290:LYS:O	1:D:294:GLU:HG3	2.21	0.41
1:C:151:VAL:CG1	1:C:292:LEU:HD13	2.48	0.41
1:C:84:GLY:HA3	1:C:147:PHE:CZ	2.56	0.41
1:C:223:PHE:CE2	1:C:227:LYS:HE3	2.56	0.41
1:B:267:MET:HA	1:B:268:PRO:HD3	1.77	0.41
1:D:9:PHE:C	1:D:11:GLU:H	2.28	0.41
1:D:147:PHE:CD2	1:D:292:LEU:HD21	2.56	0.41
1:A:163:LYS:O	1:A:164:PRO:C	2.64	0.41
1:A:253:ARG:O	1:D:97:TYR:HE1	2.04	0.41
1:B:1:MET:HB3	1:B:20:LYS:HB2	2.03	0.41
1:B:24:SER:HB3	1:B:25:TYR:H	1.52	0.41
1:B:185:LYS:HA	1:B:185:LYS:HD2	1.90	0.41
1:D:148:CYS:SG	3:D:400:BMD:OA	2.79	0.41
1:D:183:TYR:O	1:D:187:MET:HG3	2.21	0.41
1:C:53:PRO:HD3	1:C:114:TYR:CZ	2.56	0.40
1:B:49:TRP:O	1:B:50:PRO:C	2.62	0.40
1:B:64:VAL:HB	1:B:134:ILE:HD11	2.03	0.40
1:D:49:TRP:O	1:D:50:PRO:C	2.64	0.40
1:D:216:LEU:O	1:D:216:LEU:CG	2.68	0.40
1:C:9:PHE:CD1	1:C:47:GLY:HA3	2.56	0.40
1:C:182:GLN:HB3	1:C:304:VAL:HG12	2.04	0.40
1:B:163:LYS:O	1:B:164:PRO:C	2.64	0.40
1:B:173:ILE:HA	1:B:177:GLY:HA3	2.02	0.40
1:D:149:ALA:HA	1:D:176:PHE:CE2	2.56	0.40
1:A:151:VAL:HG13	1:A:292:LEU:HD13	2.04	0.40
1:C:247:ALA:O	1:C:250:SER:OG	2.39	0.40
1:C:321:ASP:H	1:C:322:ARG:HB2	1.87	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	335/339 (99%)	299 (89%)	31 (9%)	5 (2%)	8	28
1	B	335/339 (99%)	301 (90%)	27 (8%)	7 (2%)	5	21
1	C	335/339 (99%)	296 (88%)	32 (10%)	7 (2%)	5	21
1	D	335/339 (99%)	303 (90%)	26 (8%)	6 (2%)	6	25
All	All	1340/1356 (99%)	1199 (90%)	116 (9%)	25 (2%)	6	23

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	LYS
1	C	227	LYS
1	C	267	MET
1	B	215	PRO
1	B	217	LYS
1	B	218	GLU
1	B	225	LYS
1	B	227	LYS
1	D	215	PRO
1	D	227	LYS
1	C	217	LYS
1	B	100	SER
1	B	286	VAL
1	D	100	SER
1	D	217	LYS
1	D	286	VAL
1	A	50	PRO
1	A	217	LYS
1	A	286	VAL
1	C	286	VAL
1	A	199	GLU
1	C	320	PHE
1	C	50	PRO
1	D	214	ASN
1	C	101	GLY

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	267/269 (99%)	223 (84%)	44 (16%)	2	8
1	B	267/269 (99%)	226 (85%)	41 (15%)	2	9
1	C	267/269 (99%)	222 (83%)	45 (17%)	2	7
1	D	267/269 (99%)	223 (84%)	44 (16%)	2	8
All	All	1068/1076 (99%)	894 (84%)	174 (16%)	2	8

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	ILE
1	A	17	GLU
1	A	19	GLU
1	A	22	THR
1	A	28	VAL
1	A	31	ARG
1	A	42	LEU
1	A	52	LYS
1	A	54	LYS
1	A	57	LEU
1	A	69	GLU
1	A	74	VAL
1	A	75	THR
1	A	79	VAL
1	A	83	VAL
1	A	107	GLU
1	A	116	VAL
1	A	131	VAL
1	A	133	LYS
1	A	137	ASN
1	A	151	VAL
1	A	153	THR
1	A	155	LYS

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	205	LYS
1	A	216	LEU
1	A	225	LYS
1	A	251	ILE
1	A	257	CYS
1	A	259	LEU
1	A	260	VAL
1	A	271	ILE
1	A	276	LEU
1	A	285	ILE
1	A	290	LYS
1	A	304	VAL
1	A	306	THR
1	A	308	ILE
1	A	313	LEU
1	A	318	GLU
1	A	331	ARG
1	A	335	THR
1	A	336	LEU
1	C	8	GLN
1	C	15	ILE
1	C	22	THR
1	C	24	SER
1	C	33	LYS
1	C	40	THR
1	C	52	LYS
1	C	57	LEU
1	C	69	GLU
1	C	74	VAL
1	C	75	THR
1	C	83	VAL
1	C	107	GLU
1	C	108	HIS
1	C	133	LYS
1	C	137	ASN
1	C	148	CYS
1	C	151	VAL
1	C	153	THR
1	C	155	LYS
1	C	189	LEU
1	C	205	LYS

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Mol	Chain	Res	Type
1	C	216	LEU
1	C	218	GLU
1	C	222	LYS
1	C	225	LYS
1	C	244	PHE
1	C	253	ARG
1	C	259	LEU
1	C	260	VAL
1	C	265	GLU
1	C	267	MET
1	C	271	ILE
1	C	276	LEU
1	C	281	ILE
1	C	285	ILE
1	C	292	LEU
1	C	306	THR
1	C	308	ILE
1	C	313	LEU
1	C	324	LEU
1	C	325	LYS
1	C	331	ARG
1	C	335	THR
1	C	336	LEU
1	B	2	LYS
1	B	10	LYS
1	B	17	GLU
1	B	22	THR
1	B	33	LYS
1	B	57	LEU
1	B	70	VAL
1	B	74	VAL
1	B	83	VAL
1	B	100	SER
1	B	103	GLU
1	B	104	THR
1	B	107	GLU
1	B	137	ASN
1	B	151	VAL
1	B	153	THR
1	B	155	LYS
1	B	179	VAL
1	B	189	LEU

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Mol	Chain	Res	Type
1	B	205	LYS
1	B	216	LEU
1	B	227	LYS
1	B	241	LYS
1	B	251	ILE
1	B	253	ARG
1	B	259	LEU
1	B	260	VAL
1	B	265	GLU
1	B	269	ILE
1	B	276	LEU
1	B	285	ILE
1	B	288	THR
1	B	304	VAL
1	B	305	LYS
1	B	306	THR
1	B	313	LEU
1	B	318	GLU
1	B	324	LEU
1	B	325	LYS
1	B	335	THR
1	B	336	LEU
1	D	15	ILE
1	D	27	GLU
1	D	33	LYS
1	D	42	LEU
1	D	52	LYS
1	D	54	LYS
1	D	57	LEU
1	D	67	VAL
1	D	74	VAL
1	D	79	VAL
1	D	83	VAL
1	D	100	SER
1	D	104	THR
1	D	107	GLU
1	D	115	SER
1	D	137	ASN
1	D	151	VAL
1	D	153	THR
1	D	155	LYS
1	D	170	ILE

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Mol	Chain	Res	Type
1	D	179	VAL
1	D	189	LEU
1	D	205	LYS
1	D	212	VAL
1	D	225	LYS
1	D	227	LYS
1	D	239	VAL
1	D	244	PHE
1	D	251	ILE
1	D	253	ARG
1	D	259	LEU
1	D	260	VAL
1	D	267	MET
1	D	271	ILE
1	D	276	LEU
1	D	285	ILE
1	D	304	VAL
1	D	306	THR
1	D	315	LYS
1	D	318	GLU
1	D	325	LYS
1	D	328	ILE
1	D	332	VAL
1	D	336	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	111	ASN
1	A	245	GLN
1	A	249	ASN
1	A	293	GLN
1	A	317	ASN
1	C	111	ASN
1	C	317	ASN
1	B	111	ASN
1	B	293	GLN
1	B	311	GLN
1	D	109	GLN
1	D	111	ASN
1	D	214	ASN

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Mol	Chain	Res	Type
1	D	249	ASN
1	D	277	ASN
1	D	293	GLN

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	C	342	-	4,4,4	0.28	0	6,6,6	0.51	0
4	SO4	A	342	-	4,4,4	0.31	0	6,6,6	0.42	0
3	BMD	D	400	-	5,5,5	0.26	0	5,5,5	1.46	1 (20%)
3	BMD	A	600	-	5,5,5	0.42	0	5,5,5	0.55	0
3	BMD	B	500	-	5,5,5	0.15	0	5,5,5	1.34	1 (20%)
3	BMD	C	700	-	5,5,5	0.33	0	5,5,5	0.51	0
4	SO4	D	342	-	4,4,4	0.29	0	6,6,6	0.37	0
4	SO4	B	342	-	4,4,4	0.29	0	6,6,6	0.42	0

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
3	BMD	A	600	-	-	0/3/3/3	-
3	BMD	D	400	-	-	0/3/3/3	-
3	BMD	C	700	-	-	0/3/3/3	-
3	BMD	B	500	-	-	1/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	BMD	C2-C1-CA	-3.22	108.33	113.19
3	B	500	BMD	C2-C1-CA	-2.57	109.32	113.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	500	BMD	CA-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	400	BMD	2	0
3	A	600	BMD	2	0
3	B	500	BMD	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	337/339 (99%)	-1.56	0 100 100	15, 37, 59, 64	0
1	B	337/339 (99%)	-1.59	0 100 100	15, 37, 58, 64	0
1	C	337/339 (99%)	-1.57	0 100 100	16, 37, 59, 64	0
1	D	337/339 (99%)	-1.60	0 100 100	15, 37, 58, 64	0
All	All	1348/1356 (99%)	-1.58	0 100 100	15, 37, 58, 64	0

There are no RSRZ outliers to report.

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
4	SO4	A	342	5/5	0.98	0.05	102,103,103,104	0
4	SO4	C	342	5/5	0.98	0.06	103,104,105,105	0
4	SO4	D	342	5/5	0.98	0.05	90,91,92,92	0
3	BMD	C	700	6/6	0.99	0.06	26,29,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	342	5/5	0.99	0.04	86,86,87,87	0
3	BMD	A	600	6/6	0.99	0.05	25,28,28,29	0
2	ZN	D	340	1/1	1.00	0.01	43,43,43,43	0
2	ZN	D	341	1/1	1.00	0.01	31,31,31,31	0
2	ZN	A	340	1/1	1.00	0.01	50,50,50,50	0
2	ZN	A	341	1/1	1.00	0.01	31,31,31,31	0
3	BMD	B	500	6/6	1.00	0.06	38,39,39,40	0
3	BMD	D	400	6/6	1.00	0.04	35,36,36,37	0
2	ZN	C	340	1/1	1.00	0.01	48,48,48,48	0
2	ZN	C	341	1/1	1.00	0.01	32,32,32,32	0
2	ZN	B	340	1/1	1.00	0.01	39,39,39,39	0
2	ZN	B	341	1/1	1.00	0.01	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.