



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:02 PM UTC

PDB ID : 7ZSC / pdb_00007zsc
Title : Crystal structure of the heterodimeric human C-P4H-II with truncated alpha subunit (C-P4H-II delta281)
Authors : Lebedev, A.; Koski, M.K.; Wierenga, R.K.; Murthy, A.V.; Sulu, R.
Deposited on : 2022-05-06
Resolution : 3.85 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

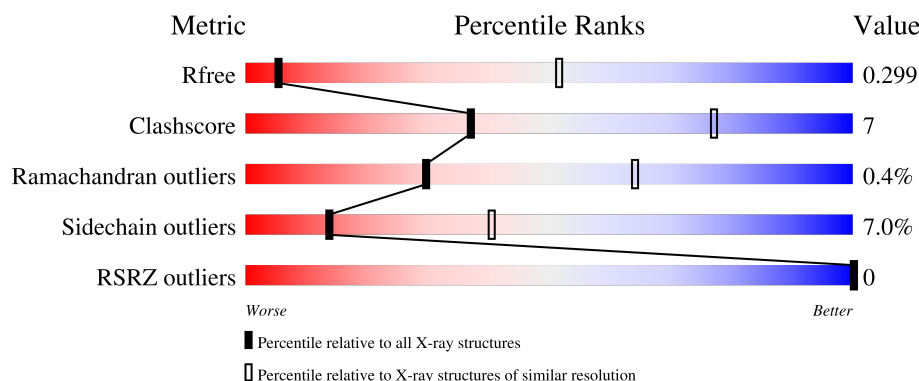
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	262	
1	B	262	
2	C	492	
2	D	492	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11098 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 Prolyl 4-hydroxylase subunit alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1920	1213	349	350	8			
1	B	233	Total	C	N	O	S	0	1	0
			1897	1198	347	344	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	MET	-	initiating methionine	UNP O15460
A	275	HIS	-	expression tag	UNP O15460
A	276	HIS	-	expression tag	UNP O15460
A	277	HIS	-	expression tag	UNP O15460
A	278	HIS	-	expression tag	UNP O15460
A	279	HIS	-	expression tag	UNP O15460
A	280	HIS	-	expression tag	UNP O15460
A	281	MET	-	expression tag	UNP O15460
B	274	MET	-	initiating methionine	UNP O15460
B	275	HIS	-	expression tag	UNP O15460
B	276	HIS	-	expression tag	UNP O15460
B	277	HIS	-	expression tag	UNP O15460
B	278	HIS	-	expression tag	UNP O15460
B	279	HIS	-	expression tag	UNP O15460
B	280	HIS	-	expression tag	UNP O15460
B	281	MET	-	expression tag	UNP O15460

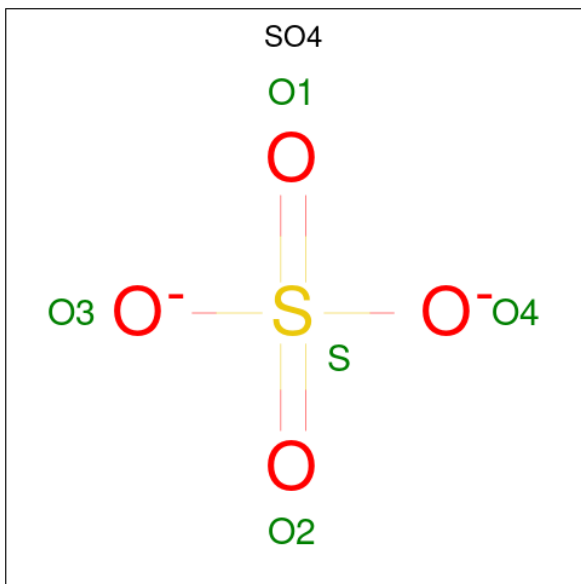
- Molecule 2 is a protein called Protein disulfide-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	456	Total	C	N	O	S	0	0	0
			3631	2329	593	700	9			
2	D	458	Total	C	N	O	S	0	0	0
			3640	2334	595	702	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	MET	-	initiating methionine	UNP P07237
D	17	MET	-	initiating methionine	UNP P07237

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

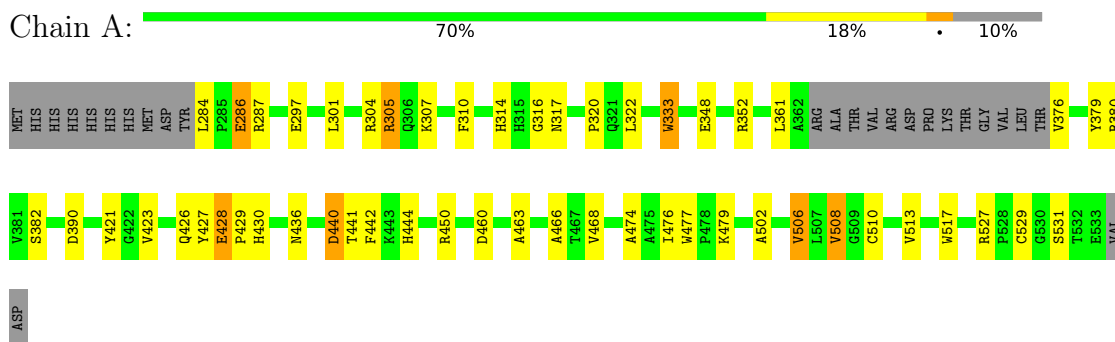


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

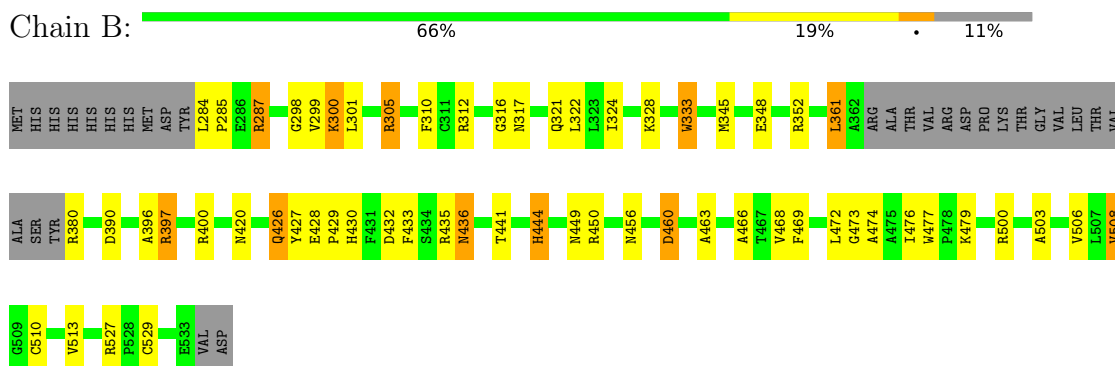
3 Residue-property plots [i](#)

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.

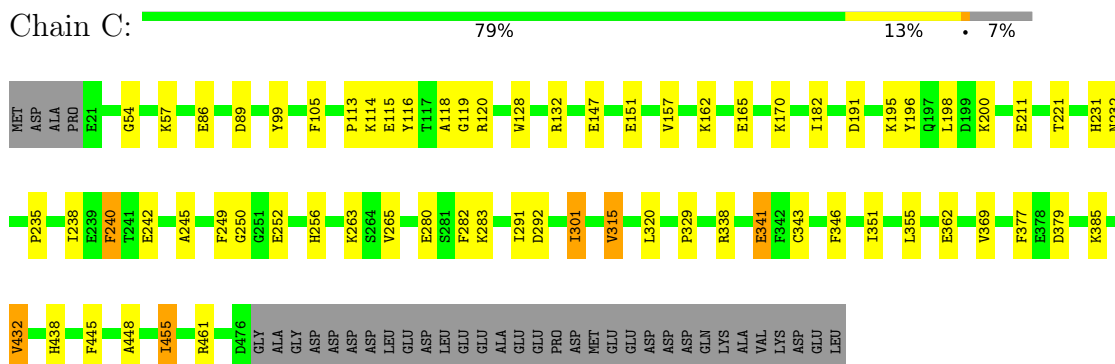
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-2



- Molecule 1: Prolyl 4-hydroxylase subunit alpha-2



- Molecule 2: Protein disulfide-isomerase



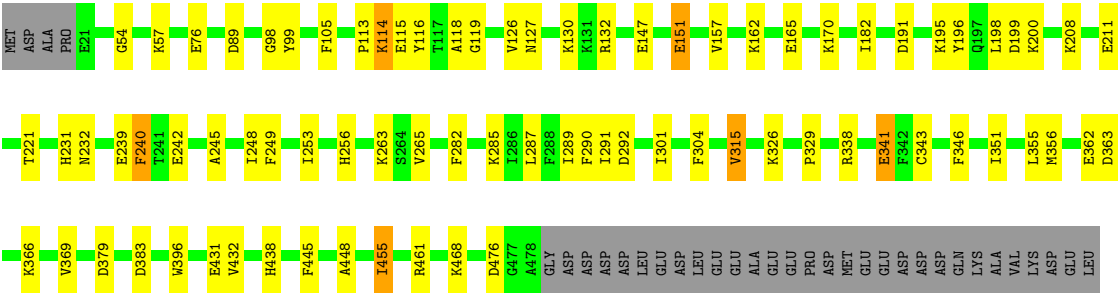
● Molecule 2: Protein disulfide-isomerase

Chain D:

77%

15%

7%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	252.88Å 252.88Å 89.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.69 – 3.85 46.69 – 3.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.69-3.85) 99.7 (46.69-3.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.244 , 0.278 0.261 , 0.299	Depositor DCC
R_{free} test set	1992 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	220.6	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11098	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: 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	0.81	0/1970	1.18	12/2665 (0.5%)
1	B	0.83	0/1950	1.19	10/2637 (0.4%)
2	C	0.69	0/3715	1.08	6/5016 (0.1%)
2	D	0.72	0/3724	1.10	7/5028 (0.1%)
All	All	0.75	0/11359	1.12	35/15346 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	314	HIS	CA-C-N	6.68	134.40	121.18
1	A	314	HIS	C-N-CA	6.68	134.40	121.18
1	A	531	SER	CA-C-N	6.43	133.83	121.54
1	A	531	SER	C-N-CA	6.43	133.83	121.54
1	A	460	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	317	ASN	CA-C-N	6.28	131.52	122.35
1	A	317	ASN	C-N-CA	6.28	131.52	122.35
1	B	435	ARG	CA-C-N	5.90	128.46	120.38
1	B	435	ARG	C-N-CA	5.90	128.46	120.38
1	A	286	GLU	N-CA-C	-5.89	105.10	112.93
1	B	317	ASN	CA-C-N	5.80	130.82	122.35
1	B	317	ASN	C-N-CA	5.80	130.82	122.35
1	B	436	ASN	CA-CB-CG	5.78	118.38	112.60
2	C	250	GLY	CA-C-N	5.67	126.94	120.53
2	C	250	GLY	C-N-CA	5.67	126.94	120.53
2	D	249	PHE	CA-CB-CG	-5.65	108.15	113.80
2	C	379	ASP	CA-CB-CG	5.59	118.19	112.60
2	D	151	GLU	CB-CG-CD	5.52	121.98	112.60
2	D	379	ASP	CA-CB-CG	5.50	118.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	440	ASP	CA-C-N	5.45	131.95	121.54
1	A	440	ASP	C-N-CA	5.45	131.95	121.54
1	A	428	GLU	N-CA-C	5.33	116.53	109.93
2	D	438	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	285	PRO	CA-C-N	5.12	131.16	122.36
1	B	285	PRO	C-N-CA	5.12	131.16	122.36
1	B	396	ALA	CA-C-N	5.10	127.07	120.44
1	B	396	ALA	C-N-CA	5.10	127.07	120.44
2	C	240	PHE	CA-CB-CG	-5.10	108.70	113.80
2	C	438	HIS	CA-CB-CG	-5.09	108.71	113.80
2	D	240	PHE	CA-CB-CG	-5.08	108.72	113.80
2	D	383	ASP	CA-C-N	5.05	127.75	120.38
2	D	383	ASP	C-N-CA	5.05	127.75	120.38
2	C	151	GLU	CB-CG-CD	5.04	121.17	112.60

There are no chirality outliers.

There are no planarity outliers.

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	1920	0	1853	32	0
1	B	1897	0	1832	43	0
2	C	3631	0	3549	42	0
2	D	3640	0	3557	51	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
All	All	11098	0	10791	155	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 7.

All (155) 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:469:PHE:HB3	1:B:472:LEU:HD13	1.36	1.07
1:B:361:LEU:HD21	1:B:420:ASN:HB3	1.55	0.89
2:C:263:LYS:HZ2	2:C:292:ASP:HB2	1.39	0.87
2:D:263:LYS:HZ2	2:D:292:ASP:HB2	1.41	0.85
1:A:333:TRP:NE1	1:A:474:ALA:HB2	1.91	0.84
2:D:162:LYS:HZ2	2:D:200:LYS:HG3	1.43	0.82
2:D:147:GLU:HG3	2:D:195:LYS:NZ	1.94	0.82
2:D:162:LYS:NZ	2:D:200:LYS:HG3	1.94	0.82
2:C:346:PHE:HA	2:C:351:ILE:HG12	1.61	0.82
2:C:162:LYS:NZ	2:C:200:LYS:HG3	1.95	0.81
2:C:147:GLU:HG3	2:C:195:LYS:NZ	1.95	0.81
2:D:346:PHE:HA	2:D:351:ILE:HG12	1.60	0.81
1:B:333:TRP:HE1	1:B:474:ALA:HB2	1.49	0.77
1:A:333:TRP:HE1	1:A:474:ALA:HB2	1.51	0.76
2:C:231:HIS:HD2	2:C:232:ASN:ND2	1.87	0.73
2:C:147:GLU:HG3	2:C:195:LYS:HZ1	1.53	0.71
1:B:333:TRP:NE1	1:B:474:ALA:HB2	2.06	0.70
2:D:165:GLU:HA	2:D:170:LYS:HZ3	1.56	0.70
2:C:165:GLU:HA	2:C:170:LYS:HZ3	1.58	0.68
2:C:263:LYS:NZ	2:C:292:ASP:HB2	2.08	0.68
2:D:162:LYS:HZ2	2:D:200:LYS:CG	2.08	0.67
1:A:441:THR:HA	1:A:444:HIS:CE1	2.30	0.66
1:B:284:LEU:HB3	1:B:287:ARG:HB2	1.76	0.66
2:D:263:LYS:NZ	2:D:292:ASP:HB2	2.10	0.66
2:D:147:GLU:HG3	2:D:195:LYS:HZ3	1.59	0.65
1:A:301:LEU:HD22	1:A:305:ARG:HG2	1.78	0.64
1:B:361:LEU:HD21	1:B:420:ASN:CB	2.26	0.64
2:C:231:HIS:HD2	2:C:232:ASN:HD21	1.46	0.62
1:A:320:PRO:HB3	2:C:249:PHE:HB2	1.81	0.62
1:A:379:TYR:HE2	1:A:426:GLN:HB3	1.64	0.62
2:D:346:PHE:HB2	2:D:351:ILE:HD11	1.83	0.61
2:C:162:LYS:HZ1	2:C:200:LYS:HG3	1.65	0.61
1:B:324:ILE:HD12	2:D:304:PHE:HE2	1.66	0.61
1:B:441:THR:HB	1:B:444:HIS:CE1	2.36	0.61
1:B:305:ARG:HE	1:B:333:TRP:HZ3	1.48	0.60
2:D:147:GLU:HG3	2:D:195:LYS:HZ1	1.66	0.60
2:D:231:HIS:HD2	2:D:232:ASN:ND2	2.00	0.60
2:C:165:GLU:HA	2:C:170:LYS:HE2	1.84	0.59
2:C:346:PHE:HB2	2:C:351:ILE:HD11	1.84	0.59
2:C:162:LYS:HZ2	2:C:200:LYS:HG3	1.65	0.59
1:B:441:THR:HG22	1:B:444:HIS:CE1	2.39	0.58
2:C:165:GLU:HA	2:C:170:LYS:NZ	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:338:ARG:HA	2:D:341:GLU:CG	2.33	0.58
2:C:263:LYS:HZ2	2:C:292:ASP:CB	2.16	0.58
2:C:338:ARG:HA	2:C:341:GLU:CG	2.33	0.58
2:D:165:GLU:HA	2:D:170:LYS:NZ	2.18	0.58
1:A:333:TRP:CD1	1:A:474:ALA:HB2	2.38	0.58
2:C:235:PRO:HG2	2:C:238:ILE:HG12	1.85	0.57
1:B:441:THR:HA	1:B:444:HIS:ND1	2.19	0.57
2:D:445:PHE:HB3	2:D:455:ILE:HG23	1.86	0.57
2:D:468:LYS:HE2	2:D:476:ASP:HB3	1.85	0.57
2:C:445:PHE:HB3	2:C:455:ILE:HG23	1.86	0.57
2:D:338:ARG:HA	2:D:341:GLU:HG2	1.86	0.56
2:D:240:PHE:CE1	2:D:245:ALA:HB2	2.40	0.56
1:B:472:LEU:HD12	1:B:472:LEU:N	2.20	0.56
2:D:151:GLU:HA	2:D:208:LYS:HZ1	1.70	0.56
2:D:165:GLU:HA	2:D:170:LYS:HE2	1.85	0.56
2:C:165:GLU:HA	2:C:170:LYS:CE	2.36	0.56
2:C:338:ARG:HA	2:C:341:GLU:HG2	1.87	0.55
1:A:477:TRP:NE1	1:B:508:VAL:HG11	2.21	0.55
1:A:508:VAL:HG11	1:B:477:TRP:NE1	2.22	0.55
2:C:256:HIS:CD2	2:C:320:LEU:HD11	2.41	0.55
2:C:280:GLU:O	2:C:283:LYS:HE2	2.07	0.55
1:B:427:TYR:HB3	1:B:503:ALA:O	2.07	0.54
2:D:356:MET:HE2	2:D:431:GLU:HG3	1.90	0.54
1:B:299:VAL:HG11	1:B:473:GLY:HA3	1.89	0.54
1:B:397:ARG:NH1	1:B:400:ARG:HH22	2.05	0.54
2:D:165:GLU:HA	2:D:170:LYS:CE	2.38	0.54
1:A:477:TRP:CE2	1:B:508:VAL:HG11	2.43	0.54
1:B:310:PHE:CE1	2:D:461:ARG:NH2	2.76	0.53
1:A:442:PHE:HZ	1:A:450:ARG:HH21	1.56	0.53
2:C:54:GLY:HA2	2:C:57:LYS:HE3	1.91	0.53
1:A:427:TYR:HE1	1:A:430:HIS:HE1	1.57	0.52
2:D:263:LYS:HZ2	2:D:292:ASP:CB	2.17	0.52
2:D:240:PHE:HD2	2:D:291:ILE:HD12	1.75	0.52
2:D:54:GLY:HA2	2:D:57:LYS:HE3	1.92	0.52
2:C:147:GLU:HG3	2:C:195:LYS:HZ3	1.74	0.52
2:D:253:ILE:HG23	2:D:256:HIS:NE2	2.25	0.52
2:D:256:HIS:CE1	2:D:287:LEU:HB3	2.45	0.52
1:A:316:GLY:HA3	1:A:322:LEU:HD12	1.91	0.51
1:A:423:VAL:HG22	1:A:506:VAL:HG22	1.93	0.51
2:D:346:PHE:HA	2:D:351:ILE:CG1	2.39	0.50
2:D:363:ASP:HA	2:D:366:LYS:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TYR:HE1	1:A:430:HIS:CE1	2.30	0.50
2:C:157:VAL:HG23	2:C:182:ILE:HG21	1.94	0.49
2:D:157:VAL:HG23	2:D:182:ILE:HG21	1.94	0.49
2:D:126:VAL:O	2:D:130:LYS:HG2	2.12	0.49
2:D:239:GLU:HB3	2:D:290:PHE:CZ	2.47	0.49
1:A:284:LEU:HG	1:A:287:ARG:H	1.78	0.49
1:B:429:PRO:HB2	1:B:500:ARG:HE	1.77	0.49
1:B:380:ARG:NE	1:B:426:GLN:HG3	2.29	0.48
1:A:466:ALA:HB2	1:A:477:TRP:CZ3	2.49	0.48
1:A:423:VAL:HA	1:A:506:VAL:HG13	1.96	0.48
1:B:328:LYS:HB3	2:D:396:TRP:CZ3	2.49	0.48
2:C:346:PHE:HA	2:C:351:ILE:CG1	2.39	0.48
1:B:441:THR:CA	1:B:444:HIS:ND1	2.77	0.47
2:C:128:TRP:CZ2	2:C:132:ARG:NE	2.82	0.47
1:B:432:ASP:O	1:B:450:ARG:HD2	2.14	0.47
2:D:240:PHE:HE1	2:D:245:ALA:HB2	1.78	0.47
1:B:441:THR:CB	1:B:444:HIS:CE1	2.98	0.47
1:A:310:PHE:CE1	2:C:461:ARG:NH2	2.83	0.47
2:C:377:PHE:CD2	2:C:432:VAL:HG21	2.50	0.47
2:C:162:LYS:HZ2	2:C:200:LYS:CG	2.27	0.46
1:A:333:TRP:CD1	1:A:474:ALA:CB	2.99	0.46
1:B:466:ALA:HB2	1:B:477:TRP:CZ3	2.51	0.46
1:B:441:THR:CG2	1:B:444:HIS:CE1	2.99	0.46
1:B:433:PHE:HB2	1:B:449:ASN:ND2	2.31	0.46
2:D:256:HIS:HE1	2:D:287:LEU:HD23	1.81	0.46
1:B:463:ALA:HB3	1:B:508:VAL:HG12	1.97	0.45
2:C:240:PHE:CE1	2:C:245:ALA:HB2	2.51	0.45
1:A:463:ALA:HB3	1:A:508:VAL:HG12	1.99	0.45
2:D:132:ARG:NE	2:D:132:ARG:HA	2.30	0.45
2:C:338:ARG:O	2:C:341:GLU:HG3	2.17	0.44
1:A:348:GLU:HG3	1:A:352:ARG:HE	1.82	0.44
1:B:441:THR:HG22	1:B:444:HIS:ND1	2.33	0.44
1:B:463:ALA:HB3	1:B:508:VAL:CG1	2.48	0.44
1:A:466:ALA:HB2	1:A:477:TRP:CE3	2.53	0.44
2:C:315:VAL:HG23	2:C:329:PRO:HG3	1.99	0.44
1:B:284:LEU:HD23	1:B:287:ARG:HB2	1.98	0.43
2:D:338:ARG:O	2:D:341:GLU:HG3	2.18	0.43
1:B:529:CYS:O	2:D:98:GLY:HA2	2.18	0.43
2:D:105:PHE:CE2	2:D:113:PRO:HB3	2.53	0.43
2:D:248:ILE:HG21	2:D:289:ILE:HD11	2.01	0.43
1:A:382:SER:HB2	1:A:421:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLY:HA3	1:B:322:LEU:HD12	2.01	0.43
1:B:348:GLU:HG3	1:B:352:ARG:HE	1.83	0.43
2:D:114:LYS:HA	2:D:114:LYS:HD2	1.84	0.43
2:C:105:PHE:CE2	2:C:113:PRO:HB3	2.54	0.42
2:D:315:VAL:HG23	2:D:329:PRO:HG3	2.00	0.42
1:A:284:LEU:CD1	1:A:286:GLU:HB2	2.49	0.42
1:B:321:GLN:H	1:B:321:GLN:CD	2.27	0.42
1:B:427:TYR:HE1	1:B:430:HIS:CE1	2.37	0.42
2:C:231:HIS:CE1	2:C:283:LYS:HE3	2.54	0.42
1:A:441:THR:HA	1:A:444:HIS:ND1	2.34	0.42
2:C:116:TYR:CE1	2:C:118:ALA:HB3	2.55	0.42
2:D:127:ASN:HA	2:D:130:LYS:HG2	2.01	0.42
2:D:346:PHE:HB2	2:D:351:ILE:CD1	2.49	0.42
1:B:301:LEU:HD22	1:B:305:ARG:HB3	2.02	0.42
1:A:284:LEU:C	1:A:286:GLU:H	2.28	0.42
1:A:429:PRO:HA	1:A:502:ALA:HB2	2.02	0.41
2:C:291:ILE:HD13	2:C:301:ILE:HG12	2.02	0.41
2:D:285:LYS:HD3	2:D:285:LYS:HA	1.93	0.41
1:A:508:VAL:HG11	1:B:477:TRP:CE2	2.54	0.41
1:B:324:ILE:HD12	2:D:304:PHE:CE2	2.52	0.41
2:D:116:TYR:CE1	2:D:118:ALA:HB3	2.55	0.41
1:A:529:CYS:HB2	2:C:99:TYR:HB2	2.03	0.41
2:D:282:PHE:CZ	2:D:343:CYS:HB2	2.56	0.41
2:C:282:PHE:CZ	2:C:343:CYS:HB2	2.56	0.41
1:A:450:ARG:NH1	1:A:517:TRP:CE2	2.89	0.41
2:C:162:LYS:HZ1	2:C:200:LYS:HA	1.85	0.41
1:B:300:LYS:HD3	1:B:300:LYS:HA	1.93	0.41
1:B:529:CYS:HB2	2:D:99:TYR:HB2	2.03	0.41
2:C:120:ARG:H	2:C:120:ARG:HG3	1.67	0.40
1:A:463:ALA:HB3	1:A:508:VAL:CG1	2.51	0.40
1:B:345:MET:HE2	1:B:456:ASN:HB3	2.04	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	233/262 (89%)	221 (95%)	11 (5%)	1 (0%)	30	64
1	B	230/262 (88%)	217 (94%)	12 (5%)	1 (0%)	30	64
2	C	454/492 (92%)	445 (98%)	7 (2%)	2 (0%)	30	64
2	D	456/492 (93%)	441 (97%)	13 (3%)	2 (0%)	30	64
All	All	1373/1508 (91%)	1324 (96%)	43 (3%)	6 (0%)	30	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	GLY
2	C	119	GLY
2	D	119	GLY
2	C	448	ALA
2	D	448	ALA
1	A	297	GLU

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	202/226 (89%)	183 (91%)	19 (9%)	8	30
1	B	200/226 (88%)	179 (90%)	21 (10%)	6	25
2	C	388/419 (93%)	367 (95%)	21 (5%)	20	46
2	D	388/419 (93%)	367 (95%)	21 (5%)	20	46
All	All	1178/1290 (91%)	1096 (93%)	82 (7%)	14	40

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ARG
1	A	305	ARG

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Mol	Chain	Res	Type
1	A	307	LYS
1	A	333	TRP
1	A	361	LEU
1	A	376	VAL
1	A	380	ARG
1	A	390	ASP
1	A	428	GLU
1	A	436	ASN
1	A	440	ASP
1	A	468	VAL
1	A	476	ILE
1	A	479	LYS
1	A	506	VAL
1	A	508	VAL
1	A	510	CYS
1	A	513	VAL
1	A	527	ARG
1	B	287	ARG
1	B	300	LYS
1	B	305	ARG
1	B	312	ARG
1	B	333	TRP
1	B	361	LEU
1	B	390	ASP
1	B	397	ARG
1	B	426	GLN
1	B	428	GLU
1	B	436	ASN
1	B	444	HIS
1	B	460	ASP
1	B	468	VAL
1	B	476	ILE
1	B	479	LYS
1	B	506	VAL
1	B	508	VAL
1	B	510	CYS
1	B	513	VAL
1	B	527	ARG
2	C	86	GLU
2	C	89	ASP
2	C	114	LYS
2	C	115	GLU

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Mol	Chain	Res	Type
2	C	191	ASP
2	C	196	TYR
2	C	198	LEU
2	C	211	GLU
2	C	221	THR
2	C	242	GLU
2	C	252	GLU
2	C	265	VAL
2	C	301	ILE
2	C	315	VAL
2	C	341	GLU
2	C	355	LEU
2	C	362	GLU
2	C	369	VAL
2	C	385	LYS
2	C	432	VAL
2	C	455	ILE
2	D	76	GLU
2	D	89	ASP
2	D	114	LYS
2	D	115	GLU
2	D	191	ASP
2	D	196	TYR
2	D	198	LEU
2	D	199	ASP
2	D	211	GLU
2	D	221	THR
2	D	242	GLU
2	D	265	VAL
2	D	301	ILE
2	D	315	VAL
2	D	326	LYS
2	D	341	GLU
2	D	355	LEU
2	D	362	GLU
2	D	369	VAL
2	D	432	VAL
2	D	455	ILE

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	314	HIS
1	A	317	ASN
1	A	430	HIS
1	A	444	HIS
1	B	314	HIS
1	B	420	ASN
1	B	430	HIS
2	C	41	HIS
2	C	171	GLN
2	C	231	HIS
2	C	232	ASN
2	D	41	HIS
2	D	171	GLN
2	D	231	HIS
2	D	232	ASN
2	D	256	HIS
2	D	354	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](#)

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](#)

2 ligands 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	$\# Z > 2$
3	SO4	B	601	-	4,4,4	0.63	0	6,6,6	0.38	0
3	SO4	A	601	-	4,4,4	0.48	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 [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	237/262 (90%)	-0.74	0 100 100	10, 50, 81, 105	0
1	B	233/262 (88%)	-0.83	0 100 100	3, 43, 75, 95	1 (0%)
2	C	456/492 (92%)	-0.98	0 100 100	57, 89, 115, 132	0
2	D	458/492 (93%)	-0.92	0 100 100	52, 86, 117, 158	0
All	All	1384/1508 (91%)	-0.89	0 100 100	3, 78, 113, 158	1 (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
3	SO4	B	601	5/5	0.91	0.09	17,21,24,24	0
3	SO4	A	601	5/5	0.95	0.04	23,26,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.