



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 1FCC / pdb_00001fcc
Title : CRYSTAL STRUCTURE OF THE C2 FRAGMENT OF STREPTOCOCCAL PROTEIN G IN COMPLEX WITH THE FC DOMAIN OF HUMAN IGG
Authors : Sauer-Eriksson, A.E.; Kleywegt, G.J.; Uhlen, M.; Jones, T.A.
Deposited on : 1995-01-17
Resolution : 3.20 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
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

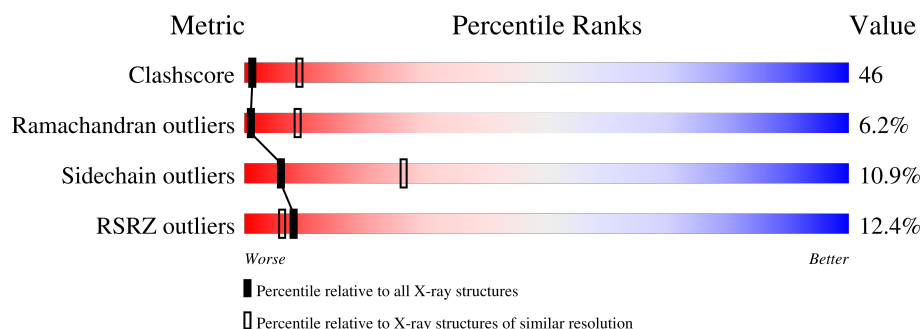
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	206	
1	B	206	
2	C	56	
2	D	56	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4180 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 IGG1 MO61 FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1656	1054	281	314	7			
1	B	206	Total	C	N	O	S	0	0	0
			1656	1054	281	314	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	conflict	UNP P01857
A	283	GLN	GLU	conflict	UNP P01857
A	294	GLN	GLU	conflict	UNP P01857
A	312	ASN	ASP	conflict	UNP P01857
A	315	ASP	ASN	conflict	UNP P01857
A	356	GLU	ASP	conflict	UNP P01857
A	358	MET	LEU	conflict	UNP P01857
B	272	GLN	GLU	conflict	UNP P01857
B	283	GLN	GLU	conflict	UNP P01857
B	294	GLN	GLU	conflict	UNP P01857
B	312	ASN	ASP	conflict	UNP P01857
B	315	ASP	ASN	conflict	UNP P01857
B	356	GLU	ASP	conflict	UNP P01857
B	358	MET	LEU	conflict	UNP P01857

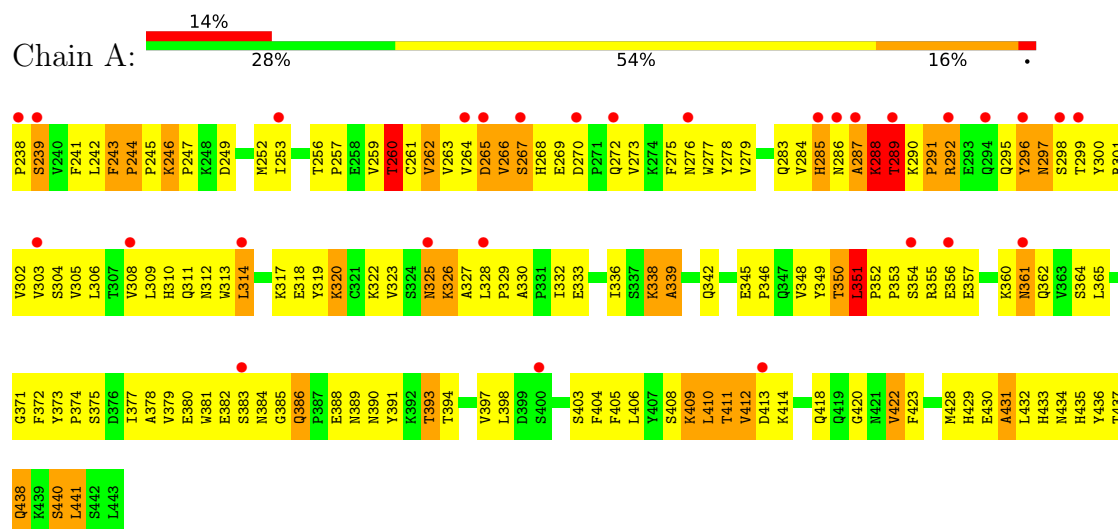
- Molecule 2 is a protein called STREPTOCOCCAL PROTEIN G (C2 FRAGMENT).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	56	Total	C	N	O	0	0	0
			434	271	67	96			
2	D	56	Total	C	N	O	0	0	0
			434	271	67	96			

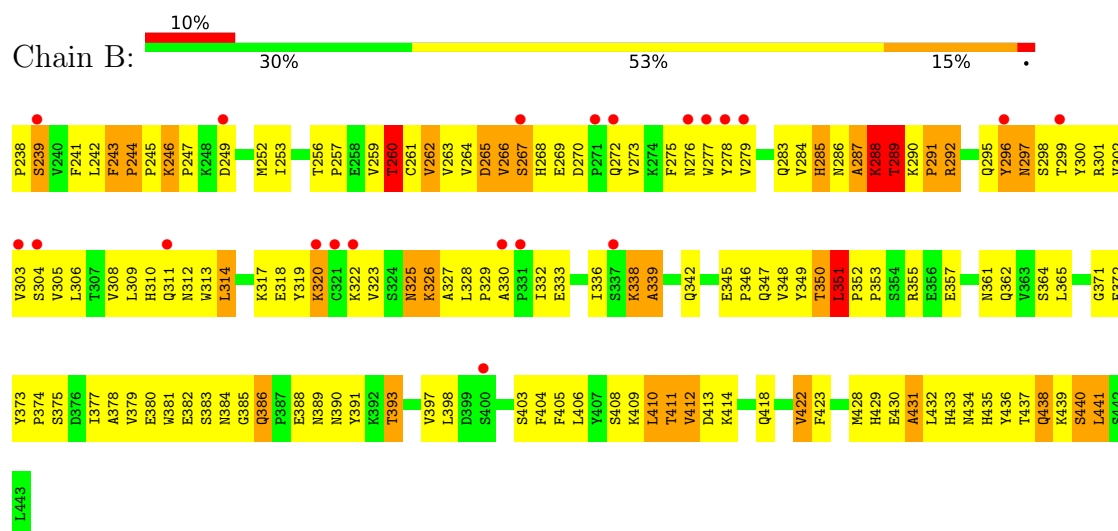
3 Residue-property plots

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: IGG1 MO61 FC

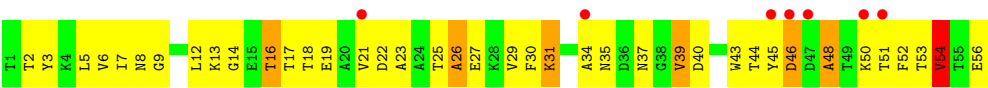


• Molecule 1: IGG1 MO61 FC

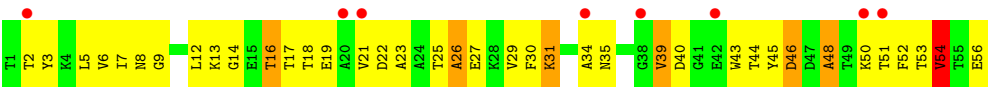


• Molecule 2: STREPTOCOCCAL PROTEIN G (C2 FRAGMENT)





● Molecule 2: STREPTOCOCCAL PROTEIN G (C2 FRAGMENT)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.60Å 110.60Å 160.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 8.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	72.0 (8.00-3.20) 66.8 (8.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.289 , 0.357 0.294 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 42.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	4180	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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	0.98	0/1702	1.41	36/2316 (1.6%)
1	B	0.98	0/1702	1.41	36/2316 (1.6%)
2	C	0.87	0/440	1.38	6/597 (1.0%)
2	D	0.87	0/440	1.38	6/597 (1.0%)
All	All	0.96	0/4284	1.40	84/5826 (1.4%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	26	ALA	N-CA-C	-11.11	98.15	112.93
2	D	26	ALA	N-CA-C	-11.11	98.15	112.93
1	B	288	LYS	N-CA-C	-10.62	88.18	110.80
1	A	288	LYS	N-CA-C	-10.61	88.20	110.80
1	B	266	VAL	N-CA-C	7.91	120.94	111.05
1	A	266	VAL	N-CA-C	7.90	120.92	111.05
1	A	275	PHE	N-CA-C	7.61	121.32	109.07
1	B	275	PHE	N-CA-C	7.60	121.31	109.07
1	B	243	PHE	CA-C-N	7.45	128.05	120.38
1	B	243	PHE	C-N-CA	7.45	128.05	120.38
1	A	243	PHE	CA-C-N	7.40	128.00	120.38
1	A	243	PHE	C-N-CA	7.40	128.00	120.38
1	A	388	GLU	N-CA-C	-7.17	101.28	110.53
1	B	388	GLU	N-CA-C	-7.16	101.30	110.53
1	A	413	ASP	N-CA-C	-6.88	100.26	110.23
1	B	413	ASP	N-CA-C	-6.84	100.30	110.23
1	A	422	VAL	CB-CA-C	-6.65	102.70	111.81
1	B	422	VAL	CB-CA-C	-6.63	102.72	111.81
2	D	48	ALA	N-CA-C	-6.62	104.06	111.28
2	C	48	ALA	N-CA-C	-6.60	104.08	111.28
2	D	14	GLY	N-CA-C	6.47	119.30	110.69
2	C	14	GLY	N-CA-C	6.45	119.26	110.69
2	D	8	ASN	N-CA-C	-6.29	102.72	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	ASN	N-CA-C	-6.29	102.72	110.65
1	A	342	GLN	CA-C-N	6.22	126.43	119.90
1	A	342	GLN	C-N-CA	6.22	126.43	119.90
1	B	342	GLN	CA-C-N	6.20	126.41	119.90
1	B	342	GLN	C-N-CA	6.20	126.41	119.90
1	B	244	PRO	CA-C-N	6.20	126.55	119.92
1	B	244	PRO	C-N-CA	6.20	126.55	119.92
1	A	244	PRO	CA-C-N	6.17	126.53	119.92
1	A	244	PRO	C-N-CA	6.17	126.53	119.92
1	A	326	LYS	N-CA-C	6.09	120.26	112.34
1	B	326	LYS	N-CA-C	6.07	120.23	112.34
1	A	412	VAL	N-CA-C	6.05	117.07	108.42
1	B	412	VAL	N-CA-C	6.03	117.04	108.42
1	B	246	LYS	CA-C-N	6.01	127.35	119.84
1	B	246	LYS	C-N-CA	6.01	127.35	119.84
1	A	246	LYS	CA-C-N	6.00	127.34	119.84
1	A	246	LYS	C-N-CA	6.00	127.34	119.84
1	A	383	SER	N-CA-C	-5.97	100.88	109.29
1	B	383	SER	N-CA-C	-5.96	100.89	109.29
1	A	386	GLN	CA-C-N	5.87	126.76	120.13
1	A	386	GLN	C-N-CA	5.87	126.76	120.13
1	B	386	GLN	CA-C-N	5.87	126.76	120.13
1	B	386	GLN	C-N-CA	5.87	126.76	120.13
1	B	409	LYS	N-CA-C	5.85	118.34	107.99
1	A	409	LYS	N-CA-C	5.84	118.33	107.99
1	B	351	LEU	CA-C-N	5.83	126.39	120.38
1	B	351	LEU	C-N-CA	5.83	126.39	120.38
1	A	351	LEU	CA-C-N	5.83	126.39	120.38
1	A	351	LEU	C-N-CA	5.83	126.39	120.38
1	A	330	ALA	N-CA-C	5.70	114.86	108.25
1	B	330	ALA	N-CA-C	5.68	114.84	108.25
1	A	320	LYS	N-CA-C	5.66	117.75	108.52
1	B	320	LYS	N-CA-C	5.65	117.73	108.52
1	A	330	ALA	CA-C-N	5.60	125.92	119.93
1	A	330	ALA	C-N-CA	5.60	125.92	119.93
1	B	330	ALA	CA-C-N	5.58	125.91	119.93
1	B	330	ALA	C-N-CA	5.58	125.91	119.93
1	A	355	ARG	N-CA-C	-5.53	105.35	111.71
1	B	355	ARG	N-CA-C	-5.53	105.35	111.71
1	B	348	VAL	N-CA-C	5.48	115.43	106.72
1	A	265	ASP	N-CA-C	-5.47	104.58	111.92
1	B	265	ASP	N-CA-C	-5.47	104.59	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	SER	N-CA-C	5.46	117.43	108.52
2	C	39	VAL	N-CA-C	-5.46	100.50	108.97
1	A	348	VAL	N-CA-C	5.46	115.40	106.72
2	D	39	VAL	N-CA-C	-5.45	100.52	108.97
1	B	364	SER	N-CA-C	5.44	117.39	108.52
1	B	431	ALA	N-CA-C	5.29	119.45	112.89
1	A	431	ALA	N-CA-C	5.29	119.44	112.89
1	A	239	SER	N-CA-C	5.13	117.04	108.99
1	B	239	SER	N-CA-C	5.13	117.04	108.99
1	B	260	THR	N-CA-C	5.10	116.83	108.52
1	A	311	GLN	N-CA-C	5.09	117.56	111.71
1	B	348	VAL	CB-CA-C	-5.09	105.17	111.32
1	A	260	THR	N-CA-C	5.08	116.79	108.52
1	A	348	VAL	CB-CA-C	-5.07	105.19	111.32
1	B	311	GLN	N-CA-C	5.06	117.53	111.71
1	B	411	THR	N-CA-C	5.04	117.97	109.95
1	A	411	THR	N-CA-C	5.02	117.94	109.95
2	C	54	VAL	CB-CA-C	-5.01	104.11	110.98
2	D	54	VAL	CB-CA-C	-5.01	104.11	110.98

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	1656	0	1630	170	1
1	B	1656	0	1630	164	0
2	C	434	0	415	40	1
2	D	434	0	415	41	0
All	All	4180	0	4090	384	2

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 46.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLU:HG3	1:B:349:TYR:CZ	1.85	1.10
1:A:371:GLY:HA2	1:A:403:SER:OG	1.73	0.89
1:A:357:GLU:HG3	1:B:349:TYR:OH	1.72	0.89
1:B:371:GLY:HA2	1:B:403:SER:OG	1.73	0.87
1:B:375:SER:HB3	1:B:404:PHE:CZ	2.10	0.86
1:A:375:SER:HB3	1:A:404:PHE:CZ	2.10	0.86
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.57	0.86
1:B:238:PRO:HA	1:B:265:ASP:HB2	1.57	0.85
1:B:338:LYS:HD2	1:B:339:ALA:O	1.77	0.85
1:B:346:PRO:HD3	1:B:429:HIS:HD2	1.42	0.84
1:A:357:GLU:CG	1:B:349:TYR:CZ	2.59	0.84
1:A:338:LYS:HD2	1:A:339:ALA:O	1.77	0.84
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.13	0.84
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.13	0.84
1:A:346:PRO:HD3	1:A:429:HIS:HD2	1.42	0.83
2:C:7:ILE:HA	2:C:54:VAL:HG23	1.62	0.82
2:D:31:LYS:HG3	2:D:43:TRP:CZ2	2.16	0.81
2:D:7:ILE:HA	2:D:54:VAL:HG23	1.61	0.81
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.64	0.80
1:A:357:GLU:HB2	1:B:349:TYR:CE1	2.16	0.80
2:C:31:LYS:HG3	2:C:43:TRP:CZ2	2.16	0.80
1:B:261:CYS:HB2	1:B:277:TRP:HZ2	1.45	0.80
2:D:44:THR:OG1	2:D:53:THR:HB	1.82	0.79
2:C:44:THR:OG1	2:C:53:THR:HB	1.82	0.79
1:A:261:CYS:HB2	1:A:277:TRP:HZ2	1.45	0.79
1:A:357:GLU:HG3	1:B:349:TYR:CE2	2.19	0.78
1:A:437:THR:HG22	1:A:438:GLN:H	1.49	0.78
2:C:3:TYR:CE2	2:C:23:ALA:HA	2.20	0.77
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.64	0.77
2:D:3:TYR:CE2	2:D:23:ALA:HA	2.20	0.77
1:B:284:VAL:HB	1:B:287:ALA:HB2	1.67	0.76
1:B:437:THR:HG22	1:B:438:GLN:H	1.49	0.76
2:C:5:LEU:HD11	2:C:54:VAL:HG22	1.67	0.76
2:D:5:LEU:HD12	2:D:6:VAL:H	1.50	0.75
1:A:242:LEU:HD23	1:A:336:ILE:HB	1.69	0.75
2:C:18:THR:HG21	2:C:29:VAL:HG11	1.69	0.75
1:A:284:VAL:HB	1:A:287:ALA:HB2	1.67	0.75
2:D:5:LEU:HD11	2:D:54:VAL:HG22	1.67	0.74
1:B:377:ILE:HG12	1:B:378:ALA:N	2.02	0.74
1:B:242:LEU:HD23	1:B:336:ILE:HB	1.69	0.74
2:C:5:LEU:HD12	2:C:6:VAL:H	1.51	0.73
1:B:257:PRO:HD3	1:B:310:HIS:NE2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:HG12	1:A:378:ALA:N	2.02	0.73
2:D:18:THR:HG21	2:D:29:VAL:HG11	1.68	0.73
1:A:257:PRO:HD3	1:A:310:HIS:NE2	2.03	0.73
1:B:393:THR:HG23	1:B:408:SER:CB	2.19	0.72
2:C:45:TYR:O	2:C:46:ASP:HB2	1.89	0.72
2:D:45:TYR:O	2:D:46:ASP:HB2	1.89	0.72
1:B:375:SER:HB3	1:B:404:PHE:CE2	2.25	0.72
1:A:393:THR:HG23	1:A:408:SER:CB	2.19	0.71
1:B:252:MET:HE3	1:B:428:MET:HE1	1.72	0.71
1:A:375:SER:HB3	1:A:404:PHE:CE2	2.25	0.71
1:A:409:LYS:HE3	1:B:405:PHE:CD2	2.25	0.71
1:A:252:MET:HE3	1:A:428:MET:HE1	1.72	0.70
1:A:308:VAL:HG12	1:A:309:LEU:N	2.07	0.70
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.74	0.70
1:B:308:VAL:HG12	1:B:309:LEU:H	1.57	0.69
1:A:245:PRO:HD2	1:A:313:TRP:CH2	2.28	0.69
1:B:245:PRO:HD2	1:B:313:TRP:CH2	2.28	0.69
2:C:5:LEU:HD12	2:C:6:VAL:N	2.07	0.69
1:B:308:VAL:HG12	1:B:309:LEU:N	2.07	0.69
1:A:357:GLU:CB	1:B:349:TYR:CZ	2.75	0.69
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.73	0.68
1:A:277:TRP:CE3	1:A:306:LEU:HD23	2.29	0.68
2:D:5:LEU:HD12	2:D:6:VAL:N	2.07	0.68
1:A:308:VAL:HG13	1:A:319:TYR:CZ	2.29	0.68
1:A:357:GLU:HB2	1:B:349:TYR:CZ	2.30	0.67
1:A:351:LEU:HD12	1:B:351:LEU:HD12	1.75	0.67
1:B:277:TRP:CE3	1:B:306:LEU:HD23	2.29	0.67
1:B:296:TYR:OH	1:B:301:ARG:HB3	1.95	0.67
1:B:346:PRO:HD3	1:B:429:HIS:CD2	2.29	0.67
1:A:295:GLN:HB2	1:A:300:TYR:HE1	1.60	0.67
1:A:296:TYR:OH	1:A:301:ARG:HB3	1.95	0.67
1:B:308:VAL:HG13	1:B:319:TYR:CZ	2.29	0.67
1:A:356:GLU:OE2	1:B:439:LYS:HE3	1.95	0.67
1:A:346:PRO:HD3	1:A:429:HIS:CD2	2.29	0.66
1:B:290:LYS:O	1:B:304:SER:HA	1.95	0.66
1:A:290:LYS:O	1:A:304:SER:HA	1.95	0.66
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.76	0.66
1:A:357:GLU:CG	1:B:349:TYR:CE2	2.78	0.66
1:A:308:VAL:HG12	1:A:309:LEU:H	1.57	0.66
1:A:360:LYS:HE3	1:B:347:GLN:OE1	1.96	0.66
1:B:352:PRO:HB2	1:B:353:PRO:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLN:HB2	1:B:300:TYR:HE1	1.60	0.66
1:B:291:PRO:HA	1:B:303:VAL:O	1.97	0.65
2:C:5:LEU:HD22	2:C:30:PHE:HB3	1.77	0.65
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.31	0.65
1:A:430:GLU:HA	1:A:435:HIS:CD2	2.32	0.65
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.76	0.65
1:A:352:PRO:HB2	1:A:353:PRO:HD2	1.77	0.65
1:A:357:GLU:CB	1:B:349:TYR:CE1	2.80	0.65
2:D:5:LEU:HD22	2:D:30:PHE:HB3	1.78	0.65
1:A:245:PRO:HD2	1:A:313:TRP:CZ2	2.33	0.64
1:A:291:PRO:HA	1:A:303:VAL:O	1.97	0.64
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.78	0.64
1:B:440:SER:O	1:B:441:LEU:HB2	1.96	0.64
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.79	0.64
1:A:397:VAL:HB	1:A:405:PHE:CE1	2.34	0.63
1:A:440:SER:O	1:A:441:LEU:HB2	1.96	0.63
1:B:397:VAL:HB	1:B:405:PHE:CE1	2.34	0.63
1:B:245:PRO:HD2	1:B:313:TRP:CZ2	2.33	0.63
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.80	0.63
1:B:393:THR:HG23	1:B:408:SER:HB2	1.81	0.63
1:A:393:THR:HG23	1:A:408:SER:HB2	1.81	0.63
1:A:279:VAL:HG23	1:A:284:VAL:HG21	1.80	0.62
1:A:239:SER:O	1:A:264:VAL:HG22	1.99	0.62
1:B:239:SER:O	1:B:264:VAL:HG22	1.99	0.62
1:B:429:HIS:ND1	1:B:430:GLU:N	2.48	0.61
2:C:3:TYR:CD2	2:C:26:ALA:HB2	2.36	0.61
1:A:357:GLU:HB2	1:B:349:TYR:CD1	2.34	0.61
2:D:3:TYR:CD2	2:D:26:ALA:HB2	2.36	0.60
1:A:429:HIS:ND1	1:A:430:GLU:N	2.48	0.60
2:D:44:THR:HG1	2:D:53:THR:HB	1.64	0.59
1:A:257:PRO:HD3	1:A:310:HIS:CD2	2.38	0.59
2:C:44:THR:HG1	2:C:53:THR:HB	1.64	0.59
2:D:16:THR:CG2	2:D:17:THR:N	2.66	0.59
1:B:414:LYS:HE3	1:B:418:GLN:NE2	2.17	0.59
1:B:393:THR:HG23	1:B:408:SER:OG	2.03	0.59
2:C:16:THR:CG2	2:C:17:THR:N	2.66	0.58
1:B:257:PRO:HD3	1:B:310:HIS:CD2	2.37	0.58
1:A:393:THR:HG23	1:A:408:SER:OG	2.03	0.58
1:B:277:TRP:HE3	1:B:306:LEU:HD23	1.67	0.58
2:D:44:THR:O	2:D:52:PHE:HA	2.03	0.58
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:HE3	1:A:418:GLN:NE2	2.17	0.58
2:C:3:TYR:HD2	2:C:26:ALA:HB2	1.68	0.58
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.85	0.58
2:C:44:THR:O	2:C:52:PHE:HA	2.03	0.58
1:B:437:THR:HG22	1:B:438:GLN:N	2.17	0.58
1:A:266:VAL:CG1	1:A:300:TYR:HB2	2.34	0.58
1:A:262:VAL:HG22	1:A:303:VAL:HG22	1.86	0.58
1:A:411:THR:HG22	1:A:412:VAL:N	2.19	0.58
1:B:262:VAL:HG22	1:B:303:VAL:HG22	1.86	0.58
1:B:411:THR:HG22	1:B:412:VAL:N	2.19	0.58
1:A:437:THR:HG22	1:A:438:GLN:N	2.17	0.57
1:B:267:SER:H	1:B:299:THR:HB	1.70	0.57
1:A:277:TRP:HE3	1:A:306:LEU:HD23	1.67	0.57
2:D:3:TYR:HD2	2:D:26:ALA:HB2	1.68	0.57
1:A:267:SER:H	1:A:299:THR:HB	1.70	0.57
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.87	0.57
1:A:259:VAL:HG23	1:A:308:VAL:CG2	2.33	0.57
1:B:266:VAL:CG1	1:B:300:TYR:HB2	2.34	0.57
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.87	0.56
2:C:39:VAL:HA	2:C:56:GLU:OE2	2.06	0.56
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.33	0.55
1:B:283:GLN:NE2	1:B:285:HIS:HD2	2.04	0.55
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.89	0.55
1:B:328:LEU:HD12	1:B:329:PRO:HD2	1.89	0.55
1:B:406:LEU:C	1:B:406:LEU:HD12	2.32	0.55
1:A:277:TRP:HA	1:A:320:LYS:O	2.07	0.55
1:A:373:TYR:CG	1:A:374:PRO:HA	2.42	0.55
1:A:406:LEU:HD12	1:A:406:LEU:C	2.32	0.55
1:B:373:TYR:CG	1:B:374:PRO:HA	2.41	0.55
1:A:283:GLN:NE2	1:A:285:HIS:HD2	2.04	0.55
1:B:295:GLN:HB2	1:B:300:TYR:CE1	2.42	0.55
2:D:39:VAL:HA	2:D:56:GLU:OE2	2.06	0.55
1:B:379:VAL:HG12	1:B:380:GLU:N	2.21	0.54
1:B:276:ASN:HB3	1:B:278:TYR:CE1	2.42	0.54
1:A:276:ASN:HB3	1:A:278:TYR:CE1	2.42	0.54
1:A:432:LEU:HD13	1:A:437:THR:OG1	2.08	0.54
1:A:356:GLU:CD	1:B:439:LYS:HE3	2.33	0.54
1:A:257:PRO:HD3	1:A:310:HIS:HE2	1.73	0.53
1:A:379:VAL:HG12	1:A:380:GLU:N	2.21	0.53
2:C:31:LYS:HA	2:C:43:TRP:CH2	2.43	0.53
1:B:277:TRP:HA	1:B:320:LYS:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:HD13	1:B:437:THR:OG1	2.08	0.53
1:B:261:CYS:CB	1:B:277:TRP:HZ2	2.19	0.53
2:C:27:GLU:O	2:C:31:LYS:HB2	2.09	0.53
1:A:295:GLN:HB2	1:A:300:TYR:CE1	2.42	0.53
2:D:27:GLU:O	2:D:31:LYS:HB2	2.08	0.53
1:A:409:LYS:CE	1:B:405:PHE:CD2	2.91	0.53
2:D:31:LYS:HA	2:D:43:TRP:CH2	2.43	0.53
1:B:257:PRO:HD3	1:B:310:HIS:HE2	1.73	0.53
1:B:264:VAL:O	1:B:265:ASP:HB2	2.09	0.53
1:B:372:PHE:CD1	1:B:404:PHE:HB2	2.44	0.53
1:A:350:THR:C	1:A:351:LEU:HD23	2.34	0.53
1:A:261:CYS:CB	1:A:277:TRP:HZ2	2.19	0.52
1:A:372:PHE:CD1	1:A:404:PHE:HB2	2.44	0.52
1:B:345:GLU:HG3	1:B:432:LEU:HD23	1.91	0.52
1:A:264:VAL:O	1:A:265:ASP:HB2	2.09	0.52
1:B:350:THR:C	1:B:351:LEU:HD23	2.34	0.52
1:A:244:PRO:HD3	1:A:336:ILE:HD11	1.92	0.52
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.91	0.52
1:B:244:PRO:HD3	1:B:336:ILE:HD11	1.92	0.52
1:A:434:ASN:ND2	2:C:35:ASN:OD1	2.44	0.51
1:B:377:ILE:HG12	1:B:378:ALA:H	1.72	0.51
1:A:389:ASN:O	1:A:391:TYR:N	2.44	0.51
2:C:40:ASP:O	2:C:56:GLU:HG2	2.11	0.51
1:A:273:VAL:CG1	1:A:323:VAL:HG13	2.41	0.51
1:A:278:TYR:CD2	1:A:283:GLN:HB2	2.46	0.51
2:D:40:ASP:O	2:D:56:GLU:HG2	2.11	0.51
2:D:25:THR:HG22	2:D:25:THR:O	2.11	0.51
1:A:279:VAL:HG23	1:A:284:VAL:CG2	2.41	0.51
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.92	0.51
1:B:273:VAL:CG1	1:B:323:VAL:HG13	2.41	0.51
1:B:411:THR:CG2	1:B:412:VAL:N	2.74	0.51
1:A:288:LYS:C	1:A:289:THR:OG1	2.55	0.51
1:B:243:PHE:HD2	1:B:260:THR:HG22	1.76	0.51
1:B:270:ASP:HB3	1:B:325:ASN:HD21	1.76	0.50
1:A:266:VAL:HB	1:A:300:TYR:CB	2.42	0.50
1:A:277:TRP:CE3	1:A:306:LEU:CD2	2.94	0.50
1:B:266:VAL:HB	1:B:300:TYR:CA	2.41	0.50
1:B:279:VAL:HG23	1:B:284:VAL:CG2	2.41	0.50
1:A:246:LYS:HB2	1:A:249:ASP:OD2	2.11	0.50
1:A:320:LYS:HE2	1:A:333:GLU:HG2	1.93	0.50
2:C:12:LEU:C	2:C:12:LEU:HD12	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HB	1:A:300:TYR:CA	2.41	0.50
1:B:266:VAL:HB	1:B:300:TYR:CB	2.42	0.50
1:B:277:TRP:CE3	1:B:306:LEU:CD2	2.94	0.50
1:B:278:TYR:CD2	1:B:283:GLN:HB2	2.46	0.50
1:A:411:THR:CG2	1:A:412:VAL:N	2.74	0.50
1:B:389:ASN:O	1:B:391:TYR:N	2.44	0.50
1:A:283:GLN:NE2	1:A:285:HIS:CD2	2.79	0.50
1:A:362:GLN:HA	1:A:412:VAL:O	2.12	0.50
1:A:394:THR:HG22	1:B:397:VAL:HG21	1.94	0.50
1:B:246:LYS:HB2	1:B:249:ASP:OD2	2.11	0.50
1:B:296:TYR:OH	1:B:301:ARG:HD3	2.12	0.50
1:B:273:VAL:HG13	1:B:323:VAL:HG13	1.93	0.50
1:A:296:TYR:O	1:A:297:ASN:HB3	2.11	0.50
1:B:434:ASN:ND2	2:D:35:ASN:OD1	2.44	0.50
1:B:283:GLN:NE2	1:B:285:HIS:CD2	2.79	0.50
1:A:286:ASN:O	1:A:288:LYS:N	2.45	0.49
1:B:296:TYR:O	1:B:297:ASN:HB3	2.11	0.49
1:A:270:ASP:HB3	1:A:325:ASN:HD21	1.76	0.49
1:A:296:TYR:OH	1:A:301:ARG:HD3	2.12	0.49
1:B:320:LYS:HE2	1:B:333:GLU:HG2	1.93	0.49
1:A:377:ILE:HG12	1:A:378:ALA:H	1.72	0.49
1:B:362:GLN:HA	1:B:412:VAL:O	2.12	0.49
2:D:3:TYR:HD1	2:D:50:LYS:HB3	1.77	0.49
1:A:243:PHE:HD2	1:A:260:THR:HG22	1.76	0.49
1:A:273:VAL:HG13	1:A:323:VAL:HG13	1.93	0.49
1:A:345:GLU:HA	1:A:431:ALA:CB	2.43	0.49
2:C:12:LEU:HD12	2:C:13:LYS:N	2.27	0.49
2:C:25:THR:O	2:C:25:THR:HG22	2.11	0.49
1:A:276:ASN:CB	1:A:322:LYS:HB3	2.42	0.49
1:A:371:GLY:HA2	1:A:403:SER:CB	2.43	0.49
1:B:345:GLU:HA	1:B:431:ALA:CB	2.43	0.49
2:D:12:LEU:HD12	2:D:12:LEU:C	2.36	0.49
1:A:356:GLU:HB2	1:B:439:LYS:HZ1	1.77	0.49
1:B:371:GLY:HA2	1:B:403:SER:CB	2.43	0.49
2:C:3:TYR:HD1	2:C:50:LYS:HB3	1.77	0.49
1:A:308:VAL:CG1	1:A:309:LEU:H	2.25	0.48
1:B:286:ASN:O	1:B:288:LYS:N	2.45	0.48
1:A:351:LEU:CD1	1:B:351:LEU:HD12	2.41	0.48
1:B:266:VAL:HB	1:B:300:TYR:C	2.39	0.48
1:B:312:ASN:HB3	1:B:317:LYS:HG3	1.95	0.48
1:B:410:LEU:HG	1:B:411:THR:N	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HB	1:A:300:TYR:C	2.38	0.48
1:A:377:ILE:CG1	1:A:378:ALA:N	2.75	0.48
2:C:23:ALA:O	2:C:26:ALA:HB3	2.14	0.48
1:B:288:LYS:C	1:B:289:THR:OG1	2.55	0.48
2:D:51:THR:HG22	2:D:52:PHE:N	2.29	0.48
2:C:16:THR:HG23	2:C:17:THR:H	1.78	0.48
2:D:12:LEU:HD12	2:D:13:LYS:N	2.27	0.48
1:B:276:ASN:CB	1:B:322:LYS:HB3	2.42	0.48
1:A:357:GLU:CA	1:B:349:TYR:CE1	2.97	0.48
1:B:377:ILE:CG1	1:B:378:ALA:N	2.75	0.48
1:B:397:VAL:HB	1:B:405:PHE:CD1	2.49	0.48
1:A:286:ASN:C	1:A:288:LYS:N	2.69	0.48
2:C:51:THR:HG22	2:C:52:PHE:N	2.29	0.48
2:D:16:THR:HG23	2:D:17:THR:H	1.78	0.48
1:B:308:VAL:CG1	1:B:309:LEU:H	2.25	0.47
1:A:345:GLU:HA	1:A:431:ALA:HB3	1.96	0.47
1:A:397:VAL:HB	1:A:405:PHE:CD1	2.49	0.47
1:B:286:ASN:C	1:B:288:LYS:N	2.69	0.47
1:B:346:PRO:HB3	1:B:372:PHE:CB	2.44	0.47
1:A:272:GLN:O	1:A:325:ASN:HB2	2.14	0.47
1:B:272:GLN:O	1:B:325:ASN:HB2	2.14	0.47
2:D:23:ALA:O	2:D:26:ALA:HB3	2.14	0.47
1:A:312:ASN:HB3	1:A:317:LYS:HG3	1.95	0.47
1:A:436:TYR:CD1	1:A:437:THR:N	2.83	0.47
1:A:365:LEU:HD12	1:A:410:LEU:CD2	2.43	0.47
1:A:384:ASN:C	1:A:386:GLN:H	2.23	0.47
1:B:345:GLU:HA	1:B:431:ALA:HB3	1.96	0.47
1:B:384:ASN:C	1:B:386:GLN:H	2.23	0.47
1:A:346:PRO:HB3	1:A:372:PHE:CB	2.44	0.46
1:B:436:TYR:CD1	1:B:437:THR:N	2.83	0.46
2:D:2:THR:O	2:D:2:THR:HG22	2.15	0.46
2:C:31:LYS:O	2:C:34:ALA:HB3	2.16	0.46
1:B:308:VAL:CG1	1:B:309:LEU:N	2.76	0.46
2:D:6:VAL:O	2:D:54:VAL:HG23	2.16	0.46
1:A:308:VAL:CG1	1:A:309:LEU:N	2.76	0.46
1:B:365:LEU:HD12	1:B:410:LEU:CD2	2.44	0.46
2:D:31:LYS:O	2:D:34:ALA:HB3	2.16	0.46
1:B:252:MET:HE3	1:B:428:MET:CE	2.43	0.46
2:D:9:GLY:HA2	2:D:56:GLU:HB2	1.98	0.46
1:A:242:LEU:HD12	1:A:243:PHE:H	1.81	0.45
1:A:291:PRO:O	1:A:292:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:HG	1:A:411:THR:N	2.22	0.45
2:C:6:VAL:O	2:C:54:VAL:HG23	2.16	0.45
1:A:278:TYR:CE1	1:A:322:LYS:HD3	2.51	0.45
1:B:267:SER:OG	1:B:268:HIS:N	2.47	0.45
2:D:45:TYR:HA	2:D:51:THR:O	2.17	0.45
1:A:288:LYS:C	1:A:289:THR:HG1	2.23	0.45
2:C:9:GLY:HA2	2:C:56:GLU:HB2	1.98	0.45
2:C:45:TYR:HA	2:C:51:THR:O	2.17	0.45
1:B:253:ILE:N	2:D:27:GLU:OE2	2.49	0.45
1:B:278:TYR:CE1	1:B:322:LYS:HD3	2.51	0.45
2:C:2:THR:HG22	2:C:2:THR:O	2.15	0.45
1:A:397:VAL:HG12	1:A:398:LEU:N	2.32	0.45
1:B:375:SER:HB3	1:B:404:PHE:CE1	2.50	0.45
1:A:357:GLU:HA	1:B:349:TYR:CE1	2.52	0.44
1:B:242:LEU:HD12	1:B:243:PHE:H	1.81	0.44
1:B:291:PRO:O	1:B:292:ARG:HB2	2.16	0.44
1:A:351:LEU:HD12	1:B:351:LEU:CD1	2.44	0.44
2:C:30:PHE:O	2:C:31:LYS:C	2.61	0.44
1:B:433:HIS:O	1:B:434:ASN:HB2	2.16	0.44
1:B:314:LEU:HD21	1:B:435:HIS:NE2	2.32	0.44
1:A:291:PRO:O	1:A:292:ARG:CB	2.65	0.44
1:B:241:PHE:HE2	1:B:264:VAL:HG21	1.83	0.44
1:A:267:SER:OG	1:A:268:HIS:N	2.47	0.44
1:A:288:LYS:O	1:A:289:THR:OG1	2.33	0.44
1:A:338:LYS:O	1:A:339:ALA:C	2.61	0.44
1:B:266:VAL:CB	1:B:300:TYR:HB2	2.48	0.44
1:B:430:GLU:HA	1:B:435:HIS:HD2	1.83	0.44
1:B:338:LYS:O	1:B:339:ALA:C	2.61	0.43
1:B:365:LEU:HD11	1:B:423:PHE:CD2	2.53	0.43
1:A:314:LEU:HD21	1:A:435:HIS:NE2	2.32	0.43
1:A:373:TYR:HA	1:A:374:PRO:C	2.43	0.43
1:B:373:TYR:HA	1:B:374:PRO:C	2.43	0.43
1:B:291:PRO:O	1:B:292:ARG:CB	2.65	0.43
1:A:375:SER:HB3	1:A:404:PHE:CE1	2.50	0.43
1:A:433:HIS:O	1:A:434:ASN:HB2	2.16	0.43
2:D:30:PHE:O	2:D:31:LYS:C	2.61	0.43
1:A:246:LYS:O	1:A:249:ASP:N	2.52	0.43
1:A:308:VAL:HG13	1:A:319:TYR:CE2	2.54	0.43
1:B:308:VAL:HG13	1:B:319:TYR:CE2	2.54	0.43
1:A:365:LEU:HD11	1:A:423:PHE:CD2	2.53	0.43
1:B:397:VAL:HG12	1:B:398:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:THR:HG23	2:D:17:THR:N	2.34	0.43
1:A:253:ILE:HG12	2:C:43:TRP:HB2	2.00	0.43
2:C:16:THR:HG23	2:C:17:THR:N	2.34	0.43
1:A:354:SER:CB	1:B:349:TYR:HB3	2.49	0.43
1:A:241:PHE:HE2	1:A:264:VAL:HG21	1.83	0.42
2:C:51:THR:HG22	2:C:52:PHE:H	1.84	0.42
1:B:253:ILE:HG12	2:D:43:TRP:HB2	2.00	0.42
2:D:31:LYS:HG3	2:D:43:TRP:CH2	2.53	0.42
1:A:252:MET:HE3	1:A:428:MET:CE	2.43	0.42
1:A:253:ILE:HD12	1:A:253:ILE:N	2.34	0.42
1:A:266:VAL:CB	1:A:300:TYR:HB2	2.48	0.42
2:C:46:ASP:OD1	2:C:48:ALA:HB3	2.20	0.42
1:B:253:ILE:N	1:B:253:ILE:HD12	2.34	0.42
1:A:356:GLU:HB2	1:B:439:LYS:NZ	2.35	0.42
2:C:31:LYS:HG3	2:C:43:TRP:CH2	2.53	0.42
1:B:290:LYS:HA	1:B:291:PRO:HD3	1.76	0.42
1:A:277:TRP:HE3	1:A:306:LEU:CD2	2.31	0.42
2:D:46:ASP:OD1	2:D:48:ALA:HB3	2.20	0.42
1:A:349:TYR:CZ	1:B:357:GLU:HG3	2.55	0.42
1:B:436:TYR:CE1	1:B:437:THR:O	2.73	0.42
1:A:263:VAL:HG21	1:A:273:VAL:HG11	2.02	0.42
1:A:308:VAL:HG13	1:A:319:TYR:OH	2.20	0.42
1:A:346:PRO:CD	1:A:429:HIS:HD2	2.23	0.42
1:B:263:VAL:HG21	1:B:273:VAL:HG11	2.02	0.42
1:B:253:ILE:O	1:B:310:HIS:HE1	2.03	0.41
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.47	0.41
2:D:43:TRP:HA	2:D:53:THR:O	2.21	0.41
1:A:253:ILE:O	1:A:310:HIS:HE1	2.03	0.41
1:A:436:TYR:CE1	1:A:437:THR:O	2.73	0.41
1:B:277:TRP:HE3	1:B:306:LEU:CD2	2.31	0.41
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.79	0.41
1:A:278:TYR:HA	1:A:283:GLN:HA	2.02	0.41
1:A:312:ASN:OD1	1:A:317:LYS:HE3	2.21	0.41
2:C:22:ASP:OD1	2:C:22:ASP:N	2.50	0.41
1:A:312:ASN:CB	1:A:317:LYS:HG3	2.51	0.41
1:A:278:TYR:OH	1:A:322:LYS:HD3	2.21	0.41
1:A:381:TRP:C	1:A:382:GLU:HG3	2.46	0.41
1:B:312:ASN:OD1	1:B:317:LYS:HE3	2.21	0.41
1:B:325:ASN:OD1	1:B:327:ALA:HB3	2.21	0.41
2:D:22:ASP:OD1	2:D:22:ASP:N	2.50	0.41
1:A:325:ASN:OD1	1:A:327:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:O	1:B:249:ASP:N	2.52	0.41
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.20	0.40
1:B:346:PRO:CD	1:B:429:HIS:HD2	2.23	0.40
1:B:381:TRP:C	1:B:382:GLU:HG3	2.46	0.40
1:A:257:PRO:HG2	1:A:308:VAL:O	2.21	0.40
1:A:290:LYS:HA	1:A:291:PRO:HD3	1.76	0.40
1:A:418:GLN:C	1:A:420:GLY:N	2.77	0.40
1:B:257:PRO:HG2	1:B:308:VAL:O	2.21	0.40
1:B:288:LYS:HB3	1:B:289:THR:H	1.70	0.40
1:A:285:HIS:C	1:A:287:ALA:H	2.29	0.40
1:A:412:VAL:HG11	1:A:423:PHE:CZ	2.57	0.40
2:C:43:TRP:HA	2:C:53:THR:O	2.21	0.40
1:B:278:TYR:OH	1:B:322:LYS:HD3	2.22	0.40
2:D:51:THR:HG22	2:D:52:PHE:H	1.84	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:OD1	1:A:361:ASN:ND2[5_544]	1.95	0.25
2:C:37:ASN:ND2	2:C:37:ASN:ND2[7_555]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/206 (99%)	171 (84%)	19 (9%)	14 (7%)	1	7
1	B	204/206 (99%)	171 (84%)	19 (9%)	14 (7%)	1	7
2	C	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	2	18
2	D	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	516/524 (98%)	432 (84%)	52 (10%)	32 (6%)	1 9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	A	291	PRO
1	A	292	ARG
1	A	298	SER
2	C	46	ASP
1	B	288	LYS
1	B	291	PRO
1	B	292	ARG
1	B	298	SER
2	D	46	ASP
1	A	285	HIS
1	A	339	ALA
1	A	385	GLY
1	A	390	ASN
1	A	441	LEU
2	C	21	VAL
1	B	285	HIS
1	B	339	ALA
1	B	385	GLY
1	B	390	ASN
1	B	441	LEU
2	D	21	VAL
1	A	289	THR
1	B	289	THR
1	A	297	ASN
1	A	438	GLN
1	B	297	ASN
1	B	438	GLN
1	A	287	ALA
1	B	287	ALA
1	A	247	PRO
1	B	247	PRO

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	193/193 (100%)	171 (89%)	22 (11%)	5	24
1	B	193/193 (100%)	171 (89%)	22 (11%)	5	24
2	C	46/46 (100%)	42 (91%)	4 (9%)	9	36
2	D	46/46 (100%)	42 (91%)	4 (9%)	9	36
All	All	478/478 (100%)	426 (89%)	52 (11%)	6	26

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	THR
1	A	260	THR
1	A	262	VAL
1	A	267	SER
1	A	269	GLU
1	A	288	LYS
1	A	289	THR
1	A	296	TYR
1	A	302	VAL
1	A	305	VAL
1	A	314	LEU
1	A	318	GLU
1	A	325	ASN
1	A	326	LYS
1	A	338	LYS
1	A	350	THR
1	A	351	LEU
1	A	361	ASN
1	A	393	THR
1	A	410	LEU
1	A	422	VAL
1	A	440	SER
2	C	16	THR
2	C	19	GLU
2	C	31	LYS
2	C	54	VAL
1	B	256	THR
1	B	260	THR

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Mol	Chain	Res	Type
1	B	262	VAL
1	B	267	SER
1	B	269	GLU
1	B	288	LYS
1	B	289	THR
1	B	296	TYR
1	B	302	VAL
1	B	305	VAL
1	B	314	LEU
1	B	318	GLU
1	B	325	ASN
1	B	326	LYS
1	B	338	LYS
1	B	350	THR
1	B	351	LEU
1	B	361	ASN
1	B	393	THR
1	B	410	LEU
1	B	422	VAL
1	B	440	SER
2	D	16	THR
2	D	19	GLU
2	D	31	LYS
2	D	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	283	GLN
1	A	285	HIS
1	A	286	ASN
1	A	310	HIS
1	A	311	GLN
1	A	390	ASN
1	A	418	GLN
1	B	276	ASN
1	B	283	GLN
1	B	285	HIS
1	B	286	ASN
1	B	310	HIS
1	B	311	GLN

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Mol	Chain	Res	Type
1	B	390	ASN
1	B	418	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](#)

There are no ligands in this entry.

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	206/206 (100%)	0.76	29 (14%) 6 5	2, 37, 83, 125	0
1	B	206/206 (100%)	0.58	21 (10%) 12 8	2, 37, 83, 125	0
2	C	56/56 (100%)	0.82	7 (12%) 8 6	2, 39, 73, 86	0
2	D	56/56 (100%)	0.65	8 (14%) 6 5	2, 39, 73, 86	0
All	All	524/524 (100%)	0.69	65 (12%) 8 6	2, 38, 83, 125	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	SER	5.1
1	A	239	SER	4.9
1	B	276	ASN	4.4
1	A	292	ARG	4.3
1	A	296	TYR	4.3
1	A	285	HIS	4.3
1	B	239	SER	4.2
1	B	267	SER	4.1
2	C	50	LYS	3.9
1	B	321	CYS	3.9
1	B	304	SER	3.6
1	B	299	THR	3.6
1	A	328	LEU	3.6
1	A	356	GLU	3.6
1	A	270	ASP	3.5
1	A	276	ASN	3.3
1	B	278	TYR	3.2
1	B	272	GLN	3.2
1	A	272	GLN	3.2
2	D	34	ALA	3.2
1	A	294	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	296	TYR	3.1
1	B	330	ALA	3.0
1	A	287	ALA	3.0
1	A	299	THR	3.0
1	B	279	VAL	2.9
1	A	253	ILE	2.9
2	D	21	VAL	2.8
2	D	20	ALA	2.8
2	D	2	THR	2.7
1	A	383	SER	2.7
1	A	303	VAL	2.6
1	B	400	SER	2.6
1	B	331	PRO	2.6
1	B	311	GLN	2.6
2	C	47	ASP	2.6
1	B	249	ASP	2.5
1	A	325	ASN	2.5
1	B	271	PRO	2.5
2	C	45	TYR	2.5
1	B	303	VAL	2.4
1	B	337	SER	2.4
1	A	400	SER	2.4
1	B	320	LYS	2.4
1	A	314	LEU	2.3
1	A	265	ASP	2.3
2	C	46	ASP	2.3
2	D	38	GLY	2.3
1	A	238	PRO	2.3
2	C	51	THR	2.2
1	A	298	SER	2.2
1	A	413	ASP	2.2
2	C	34	ALA	2.2
1	A	354	SER	2.1
1	A	361	ASN	2.1
1	A	286	ASN	2.1
2	D	51	THR	2.1
1	A	264	VAL	2.1
1	B	277	TRP	2.1
2	D	42	GLU	2.1
1	A	289	THR	2.0
1	A	308	VAL	2.0
2	C	21	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	322	LYS	2.0
2	D	50	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.